

UC Santa Barbara

UC Santa Barbara Electronic Theses and Dissertations

Title

An Ergodic Algorithm for Generating Random Knots with a Thickness Constraint

Permalink

<https://escholarship.org/uc/item/77r2g9n1>

Author

Chapman, Kyle Leland

Publication Date

2015

Peer reviewed|Thesis/dissertation

University of California
Santa Barbara

An Ergodic Algorithm for Generating Random Knots with a Thickness Constraint

A dissertation submitted in partial satisfaction
of the requirements for the degree

Doctor of Philosophy
in
Mathematics

by

Kyle Leland Chapman

Committee in charge:

Professor Ken Millett, Chair
Professor Stephen Bigelow
Professor Martin Scharlemann

June 2015

The Dissertation of Kyle Leland Chapman is approved.

Professor Stephen Bigelow

Professor Martin Scharlemann

Professor Ken Millett, Committee Chair

June 2015

An Ergodic Algorithm for Generating Random Knots with a Thickness Constraint

Copyright © 2015

by

Kyle Leland Chapman

This thesis is dedicated to my son Tristan Edward Leland
Chapman

Acknowledgements

I would like to thank and acknowledge my thesis committee, Ken Millett, Stephen Bigelow, and Martin Scharlemann, all of whom have been incredible resources for mathematical guidance and inspiration. I would also like to thank Medina Price for all of her support and wisdom. Having such good people to look up to and come to with my struggles has been invaluable. I also must thank Laura Plunkett, who proposed the problem which formed the basis for this thesis.

I want to thank my supportive family and friends, in particular my wonderful wife, who helped me get through the struggles of graduate school. I truly could not have done this without you.

Curriculum Vitæ

Kyle Leland Chapman

Education

2015	Ph.D. in Mathematics (Expected), University of California, Santa Barbara.
2011	M.A. in Mathematics, University of California, Santa Barbara.
2009	B.S. in Mathematics, California Polytechnic State University, San Luis Obispo

Research Interests

Geometric Knot Theory, Topological Knot Theory, Braid Theory, Planar Algebras, Subfactors, Combinatorics, Game Theory

Teaching Experience

Teaching Associate: University of California: Santa Barbara

Summer 2013	Methods of Proof
Summer 2012	Calculus I with Applications

Teaching Assistant: University of California: Santa Barbara

Winter 2014	Calculus for Social Sciences
Fall 2013	Linear Algebra with Applications
Spring 2013	Calculus for Social Sciences II
Winter 2013	Methods of Proof
Fall 2012	Methods of Proof
Spring 2012	Calculus with Applications II
Winter 2012	Abstract Algebra
Fall 2011	Linear Algebra with Proofs
Summer 2011	Calculus for Social Sciences II
Spring 2011	Vector Calculus II
Winter 2011	Differential Equations and Linear Algebra
Winter 2011	Vector Calculus II
Fall 2010	Methods of Proof
Summer 2010	Calculus with Applications
Spring 2010	Calculus with Applications
Winter 2010	Calculus for Social Sciences

Fall 2009 Calculus for Social Sciences

Teaching Assistant: California Polytechnic State University: San Luis Obispo

January 2008 - June 2009 Calculus, Combinatorics, Analysis

Awards and Honors

2014 Department of Mathematics Outstanding Teaching Assistant Award
2014 Department of Mathematics Graduate Student Research Grant
2008,2009 Ralph E. Weston Memorial Award for Score on Putnum

Seminar Talks

January 2014 An Alternative to the Shapley-Snow Algorithm for Completely Solving Matrix Games
 Combinatorics and Discreet Geometry Seminar: University of California Santa Barbara
October 2013 Combinatorial Games and Construction of Surreal Numbers
 Combinatorics and Discreet Geometry Seminar: University of California Santa Barbara
June 2013 A Diagramatic Presentation for the \tilde{E}_8 planar algebra
 Advancement Talk: University of California Santa Barbara
December 2010 Topological Games and the Axiom of Determinancy
 Graduate Student Topology Seminar: University of California Santa Barbara

Conferences Attended

2014 NCGOA Spring Institute, Funding Provided by Conference

Abstract

An Ergodic Algorithm for Generating Random Knots with a Thickness Constraint

by

Kyle Leland Chapman

The first algorithm for sampling the space of thick equilateral knots, as a function of thickness, will be described. This algorithm is based on previous algorithms of applying random reflections.

To prove the existence of the algorithm, we describe a method for turning any knot into the regular planar polygon using only thickness non-decreasing moves. This approach ensures that the algorithm has a positive probability of connecting any two knots with the required thickness constraint and so is ergodic. This ergodic sampling allows us to analyze the effects of thickness on properties of the geometric knot such as radius of gyration and knotting.

The data from this algorithm will show that the radius of gyration increases strongly with thickness, in that the growth exponent for radius of gyration increases with thickness. It also shows how knotting is decreased by the addition of a thickness constraint.

Contents

Curriculum Vitae	vi
Abstract	viii
1 Introduction	1
1.1 Discussion of the applications of Equilateral Knots	1
1.2 Previous Thickness Free Generation Methods	2
1.3 Thickness and Excluded Volume Problem	3
1.4 Resolution of this Obstacle	5
2 Definitions	6
2.1 Knots	6
2.2 Thickness and Curvature	8
2.3 Reflection Moves	13
3 The Algorithm	15
3.1 Convex Projections	15
3.2 Flattening the Knot	31
3.3 Convex and Planar made Regular	35
3.4 Result	39
4 Monte-Carlo Markov Chains	40
4.1 The Markov Chain	40
4.2 Forward Accessible	42
4.3 T-Chains	43
4.4 Positive Harris Recurrent	46
4.5 Ergodic	46
5 Analyzing the Data	49
5.1 Expected Number of Reflections	49
5.2 Radius of Gyration	51
5.3 Knot Types	52

6 Conclusion and Future Work	57
Bibliography	59

Chapter 1

Introduction

1.1 Discussion of the applications of Equilateral Knots

Knot theory is a discipline which has seen a large number of applications, particularly in recent years. The study of knots and links is useful for disciplines such as biology, polymer physics, and materials engineering. Many of the physical properties of structures in these fields comes from the knotting and linking of molecules rather than the actual chemical structure[1]. For example, in the case of polymeric liquids, such as dough or egg whites, the high viscosity and elasticity is attributable directly to the string like components[2]. In biology, it was first discovered that the bacteriophage ϕ X174 has DNA which has a closed loop structure[3] and since numerous other examples have been found. Further, the large structure of DNA means that even if it is technically possible for two open chain DNA strands to unlink, it is not feasible. This led to the discovery by James C. Wang of enzymes called topoisomerases which alter the knotting of DNA allowing for cellular division and indicating that the knotting of DNA impacts function [4][5]. Most attempts at proving facts about applications of knot theory have been restricted to topological knots, where we have eliminated geometric factors such as friction, rigidity, torsion, thickness, and arclength. Some work has been done to look at arclength and local homogeneity by focusing on equilateral knots of a fixed number of edges [6][7][8].

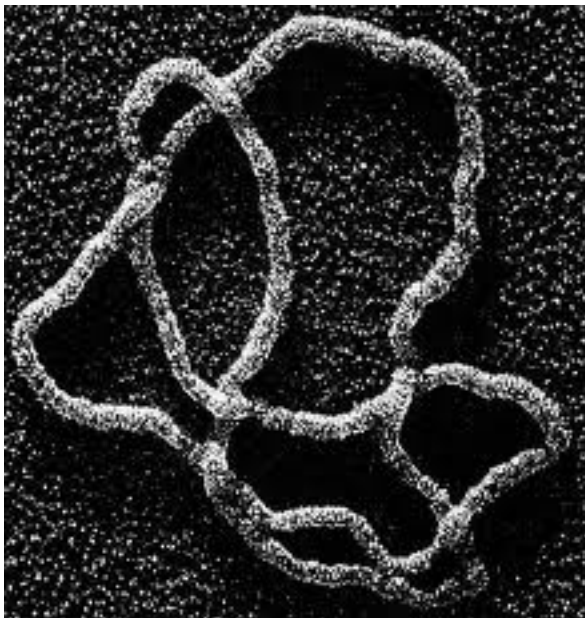


Figure 1.1: An electron micrograph of a six crossing knot in DNA[9]

Ideally, however, we would like to study knots with more of these properties included. Any information could act as a foundation upon which to make concrete statements about knots with these geometric properties. Unfortunately, even randomly sampling the space of knots with these properties poses an incredible challenge. This thesis will provide a step towards a better sampling of knots with geometric properties, specifically thickness, homogeneity, and arclength.

1.2 Previous Thickness Free Generation Methods

There are a number of methods available for the random generation of equilateral knots [10]. Because we seek to have the arc close to give a ring polygon, we can't merely generate an arbitrary random walk. Most methods come in two stages, an initialization stage, and a randomization stage. Two similar methods for initializing a closed polygon are the generalized hedgehog method, and the triangle method[10]. These involve

randomly generating sets of two or three vectors which add to zero, and then randomly ordering these vectors. Alternatively one can start just with the regular planar polygon. Any of these methods give a closed loop for a starting position, but fail to generate an arbitrary polygonal knot. From these initial positions, we can randomize by applying a sequence of moves to a starting polygon, such as polygonal folds, reflections, or crankshafts[10]. All of these moves preserve the fact that the knot closes, as well as the edge lengths and homogeneity. Unfortunately, none of these methods of direct generation or movement through knot space have been rigorously shown to give or converge to the appropriate measure on knot space. There is a method using symplectic geometry which has been shown by Cantarella and Shonkwiler to converge to the correct measure[11]. All of these generation methods allow us to sample closed knots with a fixed edge length. These methods do not, however, allow us to have any control over the thickness of the knots generated.

1.3 Thickness and Excluded Volume Problem

A knot is traditionally viewed as being an infinitesimally thin strand or loop, represented by mappings of a circle into space. In applications, however, we need knots which have a thickness, which means that they are maps of cylinders into space. This means that portions of the knot take up volume, excluding the rest of knot from occupying that space. The natural naive attempt at sampling knots with a thickness constraint is to merely generate knots using another method, such as the symplectic method, and then restrict to those samples satisfying the thickness constraint. This method is extremely ineffective in practice. This is because the probability of a knot that is randomly generated satisfying interesting thickness constraints can be very low. For example, in a sample of 10,000 random decagons, 6,990 had a thickness less than .01, compared to a maximal

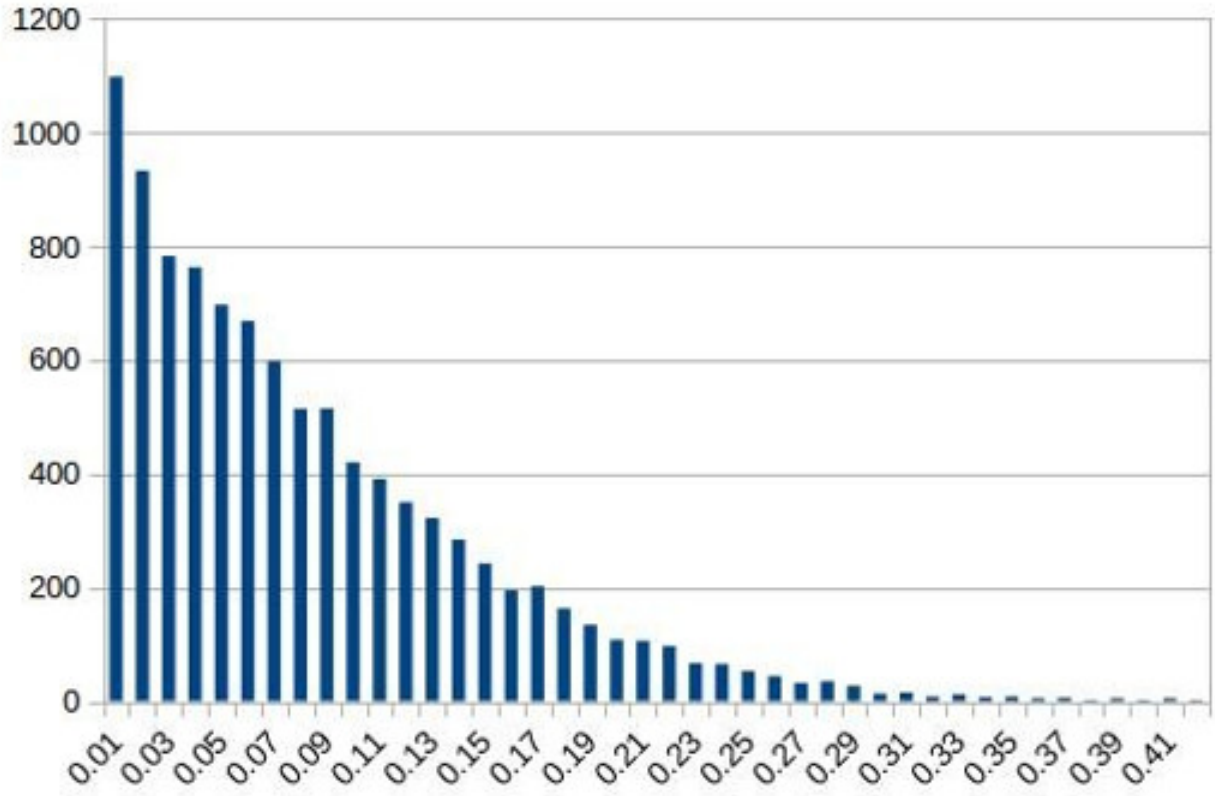


Figure 1.2: A histogram of the thicknesses of ten thousand random decagons

thickness of .1539. This problem only gets worse as the number of edges increases. Even in the case of open chains with thickness, where we can generate a chain and use that the subchain already generated will have to have satisfied the thickness constraint, we run into difficulties as it is possible for such generation methods to become trapped. This is a direct result of the problem of excluded volumes, as regions in space may become too filled with portions of the knot which were previously generated to allow for passage by a tube of the chosen thickness constraint. This returns us to a problem faced by closed chains, as you must make numerous attempts to generate each sample. Each of these methods can become extremely time consuming when trying to generate adequate sample sizes.

1.4 Resolution of this Obstacle

In this thesis, we give a method of generating knots with a thickness constraint. It allows us to check the thickness throughout the generation procedure. It is built on the standard reflection algorithm, which starts with the regular planar polygon, and applies a sequence of reflection moves to generate a random knot. We check the thickness after a specific number of reflections to make sure the thickness constraint we desire is still maintained. Verifying that this will randomly sample the whole space of knots of a given thickness is the focus of this paper. While the act of checking thickness increases computation time, this method is still an improvement over the extremely low yield of previous algorithms.

Chapter 2

Definitions

2.1 Knots

In this thesis we use the following definitions. We will be considering knots as piecewise linear equilateral polygons in 3-space, rather than the more common notion of smooth or topological knots, since the class of piecewise linear equilateral knots is more useful for simulation and applications to the study of macromolecules, and is much more tractable for computer based analysis. A knot with n edges will be defined to be a sequence of n points, called its vertexes, $\{v_i\}_{i \in \mathbb{Z}_n}$ in \mathbb{R}^3 with the property that $\|v_{i+1} - v_i\| = 1$ for each index, and for which the line segments connecting pairs of adjacent vertexes intersect in, at most, a common vertex. The indexing is in \mathbb{Z}_n so that the result is a closed loop. The space of such knots will be denoted $\text{Equ}(n)$, and be given the subset topology of \mathbb{R}^{3n} . Knots in $\text{Equ}(n)$ will be considered equivalent if they differ by an affine transformation, which is a composition of translations and rotations. These transformations are the orientation preserving component of the isometry group for \mathbb{R}^3 and so preserve all lengths and angles of the knot. This equivalence is to account for the fact that the knot properties should be independent of where the origin is or the choice of oriented orthogonal basis. An *arc* of the knot is a subsequence of the knot given by $\{v_i\}_{i=j}^k$. Due to the cyclic indexing, this corresponds to the traditional notion of a subarc of a knot.

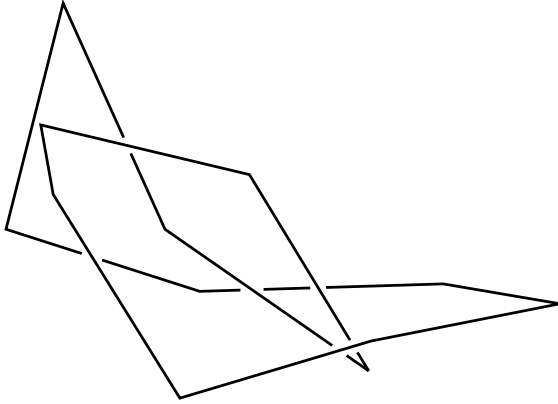


Figure 2.1: A sample random 12-gon

Given an arc $a = \{v_i\}_{i=j}^k$ we will define the complementary arc to be $a^c = \{v_i\}_{i=k}^{j+n}$.

An *edge* of a knot or arc is simply the straight line segment connecting a pair of adjacent vertexes. The realization of a knot or arc is the union of its edges as subsets of \mathbb{R}^3 . Note that the realization of an arc union the realization of the complementary arc is the realization of the whole knot. The *interior angle* at a vertex, x_i is defined to be the angle between the two vectors $v_{i+1} - v_i$ and $v_{i-1} - v_i$. This angle will be called *regular* if it equals $\pi \frac{n-2}{n}$, large if it is larger than regular and small if it is smaller than regular. The *turning angle* of a vertex is π minus the interior angle of the vertex. This gives us a means of discussing the curvature of a piecewise linear knot, as being the turning angle at a vertex.

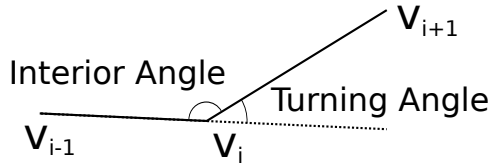


Figure 2.2: The two angles of importance at each vertex

2.2 Thickness and Curvature

The polygonal injectivity radius will be as defined by Rawdon in [12], which is chosen in such a way as to limit upon the injectivity radius of a smooth curve. Recall that for a smooth curve, the injectivity radius is the largest r such that a disk of radius r perpendicular to the curve can be centered at every point of the knot simultaneously without intersections between distinct disks. The two limiting factors to this are the curvature, which will cause close disks to intersect, and long range interactions. For this reason, there are two types of radii we must consider for polygonal knots, taking their minimum. For an equilateral knot K , the short range radius, $MinRad(K)$, is defined as the minimum over all vertexes of $d_v = \frac{1}{2} \tan(\theta_v/2)$, where θ_v is the interior angle at the vertex v . This is the maximum radius of disks which can be placed perpendicular to the midpoints of the two adjacent edges without intersection. This also means that an arc of a circle with radius d_v can be inscribed in the pair of edges adjacent to v and meeting it at the midpoints of the edge. For any radius $r < d_v$, the same can be said, except that the intersection with the edges will be closer to the vertex.

A pair of points on the knot, a, b will be called a *doubly critical pair* if a is a local extrema of the distance function to b and b is a local extrema of the distance function to a . The set of all such pairs is $DC(K)$. The long range radius is half of the doubly

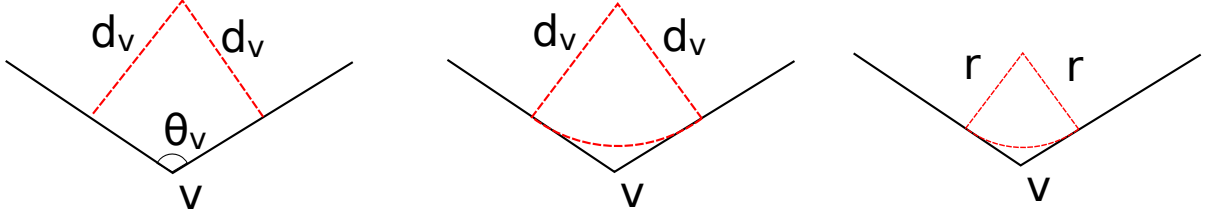


Figure 2.3: The left diagram shows the perpendicular bisectors which intersect at a distance of d_v . The middle and right diagram show inscribing an arc of a circle with radius d_v and $r < d_v$.

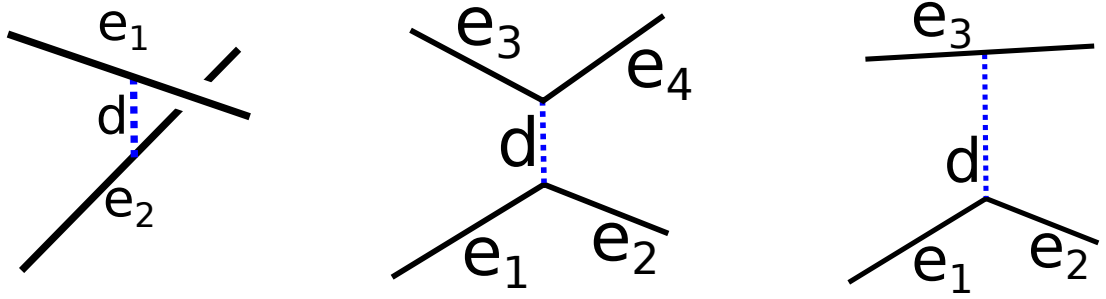


Figure 2.4: The three cases for doubly critical self distance, a pair of skew edges, a pair of vertexes, and a vertex-edge pair.

critical self distance $dcsd(K) = \min_{(a,b) \in DC(K)} (\|a - b\|)$. The *injectivity radius* is defined by $R(K) = \min(\text{MinRad}(K), dcsd(K)/2)$. As in the smooth case, *thickness* is the injectivity radius divided by the arclength. We will denote the space of equilateral knots with thickness greater than or equal to t by $Equ(n, t)$.

The *total curvature* between two points of the realization $tc(a, b)$ is the minimum over the two arcs connecting a to b of the sum of turning angles for vertexes between a and b , including the turning angles at a and/or b if either is a vertex. We will use this notion of curvature by applying Schur's theorem for sectionally smooth curves.

Theorem 1 (Schur's Theorem for Sectionally Smooth Curves [13]) *Suppose C and C^* are two sectionally smooth curves of the same length parametrized by arclength, with κ, κ^* being their curvatures within the smooth sections, α, α^* being their turning angles*

at the vertexes between smooth section and C together with its chord forming a simple convex planar curve. If $\kappa^*(s) \leq \kappa(s)$ and $\alpha^*(v) \leq \alpha(v)$, then the end to end distance of C is less than or equal to the end to end distance of C^* .

One consequence of Schur's theorem is that if we have an arbitrary curve C^* , and we do not decrease the pointwise curvatures and turning angles, that moving to a planar convex curve C cannot increase end-to-end distance. This condition of having a convex planar curve to compare to is certainly satisfied if the total curvature between points is less than or equal to π . The set of points which are separated by at least π in turning angle will be denoted $TC(K) = \{(a, b) | tc(a, b) > \pi\} \subseteq K \times K$. This definition, together with Schur's theorem, allows us to state and prove a lemma from [12] which we will use in a couple of places.

Lemma 2 *If a, b are a pair of vertexes of K on the boundary of $TC(K)$, then $\|a - b\| \geq 2MinRad(K)$.*

Proof: Let a, b be a pair of vertexes of on the boundary of $TC(K)$. The fact that a, b is on the boundary of $TC(K)$, means that the arc connecting a to b consists of vertexes v_0, v_1, \dots, v_k , with $v_0 = a, v_k = b, tc(v_0, v_{k-1}) \leq \pi$ and $tc(v_0, v_k) > \pi$. This allows us to create a planar piecewise linear equilateral curve $C = \{w_i\}_{i=-1}^{k+1}$ with w_{-1} on the negative x -axis, w_0 at the origin, and the turning angles of w_i matching the turning angles of v_i proceeding clockwise, except at w_k which proceeds parallel to the x -axis. This curve C is like the arc connecting a to b in that all turning angles are the same but it has been flattened. The fact that the total curvature including a and b is greater than or equal to π tells us that the final turning angle of C is less than or equal to the turning angle at b . Thus, since no interior angle has shrunk, $MinRad(C) \geq MinRad(K)$. Further, Schur's theorem for sectionally smooth curves tells us that if the turning angles at vertexes are not increased, the curvature at any regular point is not increased, and the resulting curve

C is convex and planar. Thus the end-to-end distance of C is greater than or equal to that of the original curve. In our case, this means that $\|a - b\| \geq \|w_k - w_0\|$. We also note that the distance between w_k and w_0 is greater than or equal to the difference in their y coordinate. By the definition of $MinRad(C)$, we can inscribe an arc of a circle whose radius is $MinRad(C)$ and whose curvature is the angle of w_i at each vertex w_i intersecting the neighboring edges no further than .5 from the vertex w_i . Replacing the neighborhood of each w_i with this arc of a circle gives us a new differentiable curve I . This curve I consists of a collection of k arcs of a circle of radius $MinRad(C)$ and total angle π , together with a collection of intermediate intervals. The curve I has an increasing y coordinate, so converting I to I^* by removing all intermediate intervals decreases the difference in y coordinate of the end-points. Finally, this allows us to observe that I^* is a circle of radius $MinRad(C)$ giving us the following.

$$\begin{aligned}
2MinRad(C) &\leq (w_k)_y - (w_0)_y \\
&\leq \|w_k - w_0\| \\
&\leq \|b - a\|
\end{aligned}$$

■

This lets us prove another lemma, from [12], that will make it much easier to determine when thickness has not been decreased. It allows us to expand our consideration from pairs of points which are doubly critical, to those which are separated by enough curvature. This is a much easier collection of points to directly compare.

Lemma 3 *For a polygonal knot K , the injectivity radius $R(K) = \min(MinRad(K), \min_{(a,b) \in TC(K)} (\|a - b\|)/2)$*

Proof: Note first that if $\min_{(a,b) \in TC(K)} (\|a - b\|)$ is achieved on the interior of

$TC(K)$, then it occurs at a doubly critical point. If it occurs on the boundary of $TC(K)$, then Lemma 2 tells us that $\|a - b\| \geq 2MinRad(K)$. This gives us two cases. In the first case, $\min_{(a,b) \in TC(K)}(\|a - b\|) = dcsd(K)$ so $\min(MinRad(K), dcsd(K)/2) = \min(MinRad(K), \min_{(a,b) \in TC(K)}(\|a - b\|)/2)$ and the result is shown. In the other case,

$$\begin{aligned} \min_{(a,b) \in TC(K)}(\|a - b\|) &\leq dcsd(K) \\ \min_{(a,b) \in TC(K)}(\|a - b\|) &\geq 2MinRad(K) \\ \Rightarrow R(K) &= MinRad(K) = \min(MinRad(K), \min_{(a,b) \in TC(K)}(\|a - b\|)/2) \end{aligned}$$

Thus, the result is shown in all cases. ■

Corollary 4 *The injectivity radius of a convex planar polygon K is $MinRad(K)$*

Proof: In a convex planar polygon K , $TC(K)$ is empty and so the minimum is determined only by the first term, $MinRad(K)$. ■

This definition of thickness has four nice properties, which indicate that it is an appropriate choice for our definition of polygonal thickness. The first three of these properties are established in [12] and [14], and the fourth is a simple but useful corollary of [12] which we will state here as Lemma 5. First, we note that if r is less than the injectivity radius of a knot K , then the r neighborhood of the realization of the knot is an embedded torus, giving a tubular neighborhood. Second, this thickness well models the situation in the smooth category, in that a sequence of polygonal knots which limit appropriately on a smooth knot, will have a thickness which limits on the smooth thickness. Third, thickness is continuous, which in particular means that $Equ(n, t)$ is compact and has $\text{int}(Equ(n, t))$ consists of knots with thickness strictly greater than t . Finally, any edge length preserving alteration of a knot which causes distance between points of its realization to have non-decreasing distance will not decrease thickness.

2.3 Reflection Moves

An arc reflection or, simply, a *reflection move* consists of making a choice of plane containing two vertexes x_i, x_j and reflecting the vertexes $\{x_k\}_{k=i}^j$ across that plane to get a new knot. For many of the planes we will choose in the next section, the full arc $\{x_k\}_{k=i}^j$ lies on one side of the plane of reflection, but this is not required for the move to be defined. If parts of the arc lie on both sides of the plane of reflection, this simply means the vertexes in the arc switch sides of the plane of reflection. We also note that reflecting an arc across a plane, and reflecting the complementary arc across the same plane differ by a reflection of the whole knot across that plane, which is an affine transformation. Thus, we may choose with each reflection move to reflect either arc connecting the chosen vertexes.

The result of a reflection move may not in general be a non-singular knot, as self-intersections may be created, but we will still consider such non-embedded curves as knots with zero thickness. We also will talk about neighborhoods of a reflection move, where the space of reflection moves on a knot is given by a disjoint union of circles. This is because each pair of vertexes defines a line which the reflection plane must contain, and the planes through a given fixed line form a circle.

Lemma 5 *If $K, K' \in Equ(n)$ and there is an arclength preserving function $f : K \rightarrow K'$ such that $d(f(a), f(b)) \geq d(a, b)$ for every pair of points $a, b \in K$, then the thickness of K' is greater than or equal to the thickness of K*

Proof: First, consider the interior angles. We will examine a pair of points, a, b , one immediately before and one immediately after a vertex, v . The distance between these two points cannot decrease, while their distance to the vertex is preserved. These quantities determine the interior angle of that vertex and show that it cannot decrease. Thus, the interior angles are all non-decreasing.

Second, we use Lemma 3 which says that rather than only checking long range thickness at points which locally minimize distance, we can look at the long range thickness between any pair of points separated by a total of π turning angles. We have already established that each interior angle is non-decreasing, which means that the turning angles are non-increasing. This tells us that if $tc(a, b) \leq \pi$ then $tc(f(a), f(b)) \leq \pi$, and so $TC(K') \subseteq f(TC(K))$. Further, since every pair of points is made no closer, we have the following

$$\begin{aligned} \min_{(a,b) \in TC(K)} (\|a - b\|) &\leq \\ \min_{(f(a), f(b)) \in TC(K')} (\|a - b\|) &\leq \\ \min_{(f(a), f(b)) \in TC(K')} (\|f(a) - f(b)\|) &= \min_{(a,b) \in TC(K')} (\|a - b\|) \end{aligned}$$

Therefore the long range thickness is non-decreasing. Thus, the result is shown. ■

Chapter 3

The Algorithm

We can consider applying random reflection moves to a knot $K \in Equ(n, t)$. Sometimes these random reflection moves will result in a new knot in $Equ(n, t)$ and sometimes it will not. We will show that if we apply random reflections, then every neighborhood of the regular planar polygon has a positive probability of being reached in finite time from every starting position, without leaving $Equ(n, t)$ for more than 6 reflections. For this, we will show that for any knot K in $Equ(n, t)$, there is a sequence of moves m_i consisting of up to 6 reflection moves each, giving a sequence of knots $\{K_i\}_0^N$ of knots also in $Equ(n, t)$ with $K = K_0$, K_N the regular planar polygon, each $K_{i+1} = m_i(K_i)$ and each m_i having an open neighborhood M_i with $m(K_i) \in Equ(n, t)$ for every $m \in M_i$.

First, we will show that there is a way of spreading out the knot so that it has a projection which is convex. We then start flattening the knot until it is planar. Finally, we will do moves to make each angle regular, resulting in the regular planar polygon.

3.1 Convex Projections

Throughout this portion of the algorithm, we would like to know that expanding the knot does not decrease the thickness. In practice, this amounts to showing the injectivity radius is not decreased, since throughout the process the arclength is preserved. We will

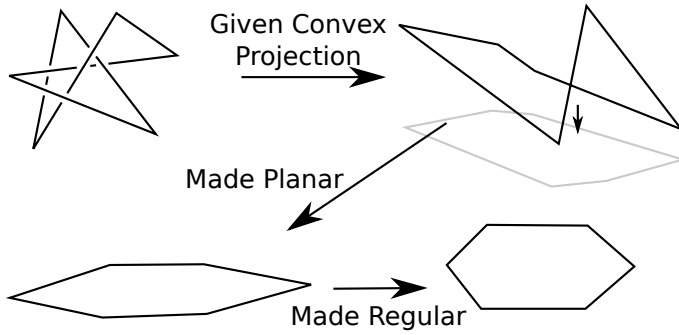


Figure 3.1: An example of three steps applied to a random hexagon

use the following lemma multiple times.

Lemma 6 *If r is a reflection move on a knot K across a plane P with P not intersecting the interior of the convex hull of K , then the thickness of $r(K)$ is no less than the thickness of K .*

Proof: By Lemma 5, it suffices to show that the distance between any two points is not decreased by r . We can also conjugate by an affine transformation, which means that without loss of generality we can choose P to be the $x-y$ plane, and K living in the upper half space. If both points are fixed or both points move, then the distance between them is unchanged, so it suffices to consider pairs of points where exactly one of the two is moved. We denote these two points (x, y, z) and (x', y', z') with $z, z' \geq 0$. Thus, the

lemma has been reduced to showing that $d((x, y, z), (x', y', z')) \leq d((x, y, z), (x', y', -z'))$.

$$z, z' \geq 0$$

$$2zz' \geq -2zz'$$

$$z^2 + 2zz' + z'^2 \geq z^2 - 2zz' + z'^2$$

$$(z + z')^2 \geq (z - z')^2$$

$$(x - x')^2 + (y - y')^2 + (z - (-z'))^2 \geq (x - x')^2 + (y - y')^2 + (z - z')^2$$

$$d((x, y, z), (x', y', -z'))^2 \geq d((x, y, z), (x', y', z'))^2$$

Thus, the distance between pairs of points is not decreased by r and so the thickness of $r(K)$ is no less than the thickness of K . ■

We now proceed with applying a sequence of reflection moves to a knot K so that some projection $p(K)$ is convex. We choose the orthogonal projection into the $x - y$ plane, giving us $p(K) \subseteq \mathbb{R}^2$. We want to choose a fixed orthogonal projection for two reasons. First, it is useful that a reflection in the plane will correspond to a reflection in space, which requires that the projection is orthogonal. Second, it is important that we have a well defined and consistent set of minimum height vertexes. This means that we may apply a rotation to the whole knot before beginning, but once we have made a choice of projection, we must stick to it. This, unfortunately, will prevent us from using arguments about general position, but such methods can be safely avoided. Because we have done nothing special to the knot beforehand, this map may be terribly non-injective and perhaps is not even an immersion. Regardless, it is a piecewise linear map into the plane, about which many results are known. Our preliminary goal will be to apply reflection moves to K so as to make $p(K)$ convex, while maintaining certain properties along the way.

We need a few definitions for this section specifically. A vertex of a polygon in \mathbb{R}^2 is *exposed* if it is also a vertex of the convex hull. A pair of vertexes is an *exposed pair* if they are both exposed and share a line which does not intersect the interior of the convex hull and which does not contain either arc connecting them. This means a reflection of one of the two arcs connecting an exposed pair of vertexes changes the polygon. We also need three notions of convexity. We will be considering a function $f : S^1 \rightarrow K \rightarrow \mathbb{R}^2$, but these definitions can be applied equally well to any piecewise linear map $f : S^1 \rightarrow \mathbb{R}^3$. The first of the definitions is that a map $f : S^1 \rightarrow \mathbb{R}^2$ is *convex* if it is an embedding onto the boundary of the convex hull of its image. We will also use a weaker notion, that a map $f : S^1 \rightarrow \mathbb{R}^2$ is *nearly convex* if its image is contained in the boundary of the convex hull of its image. A nearly convex map might run back and forth through a proper subset of the boundary of the convex hull or zig zag back and forth within an edge before continuing, but it will still be useful for our purposes. In between these two notions is the idea of a polygon being *exposed*, which means that it is nearly convex and the preimage of every exposed vertex is connected, meaning that we have eliminated the cases such as moving back and forth through a proper subset or winding about the convex hull multiple times, but we may still have zig-zagging within an edge of the boundary of the convex hull. It is also important to acknowledge that a map which is *subdimensional*, meaning the convex hull has empty interior, will automatically be nearly convex, and may be exposed. We will quote a theorem of two-dimensional geometry before proving a three dimensional analog.

3.1.1 Grünbaum-Zaks Theorem

We will be basing our argument about three dimensional knots on the following theorem.

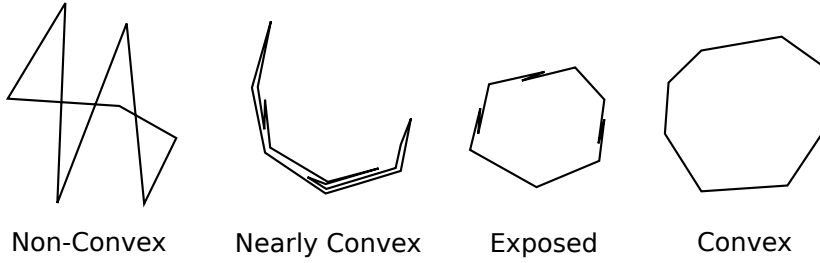


Figure 3.2: Examples of the types of convexity defined in this section. Overlapping edges are separated for clarity.

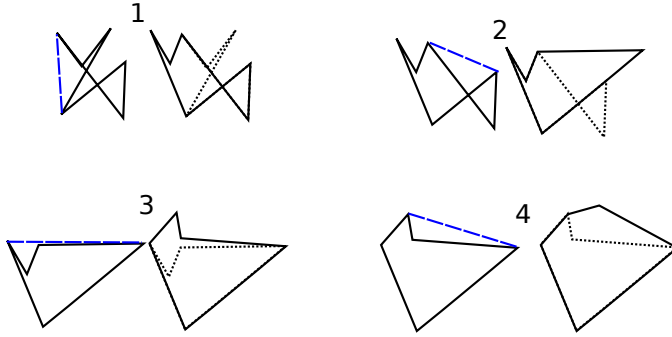


Figure 3.3: An example of a polygonal loop which can be convexified in 4 reflections. Each reflection move is shown using two figures. The left is the polygon before the reflection with a supporting line connecting exposed vertexes highlighted in blue. The tight polygon is the result of the move and shows the previous location of the moved arc as a dotted line. Note that the initial configuration includes a partial doubling back, a type of non-generic intersection which can be accounted for by the theorem.

Theorem 7 *Every polygon in the plane, not necessarily embedded, can be transformed into an exposed polygon by a finite sequence of reflections, determined at each step by an exposed pair of vertices*

This theorem was proven in 2001 by Grünbaum and Zaks[15], appearing as Theorem 3. We will use the ability to convexify polygonal loops in the plane in Theorem 16 to make the orthogonal projection of the knot into the $x - y$ plane exposed. We require the argument of this theorem which is stronger than earlier results such as the Erdős-Nagy Theorem[16], which applies to embedded polygons, because we need to be able to consider

intersections in the projection, such as multiple vertexes going to the same point, or edges intersecting in segments as in Figure 3.1.1. Our needs also require different choices of vertexes.

We prove a sequence of lemmas that, when taken together, prove the desired theorem about knots in space. We first show that if the projection of our knot isn't exposed, it has an exposed pair.

Lemma 8 *If $p(K)$ is a polygon in the plane which is not exposed, then it has an exposed pair.*

Proof: First, consider the case where $p(K)$ is not nearly convex. This means that there is some point x of $p(K)$ on the interior of $\text{conv}(p(K))$. This also means $\text{conv}(p(K))$ is not subdimensional, which means that $p(K)$ has at least three non-collinear exposed vertexes. This point x need not be a vertex of $p(K)$. From x , proceed forward to the first exposed vertex v_i . The vertex v_i has two supporting lines of $\text{conv}(p(K))$ coming out of it. The edge e_i coming out of v_i cannot lie in both, so choose a supporting line l of $\text{conv}(p(K))$ which contains v_i but does not contain e_i . This line must hit a second exposed vertex v_j . The line l then does not contain either arc connecting v_i to v_j , as it does not contain e_i and it does not contain x , and by the choice of v_i as the first exposed vertex after x , these must lie in different arcs connecting v_i to v_j . Therefore, v_i and v_j form an exposed pair.

Next, consider the case where $p(K)$ is nearly convex but not exposed. This means that there is some vertex of $\text{conv}(p(K))$ with disconnected preimage. This tells us that there are v_i, v_j with $p(v_i) = p(v_j)$ but with neither arc connecting v_i to v_j mapped to $p(v_i)$. Let l be a line which intersects $\text{conv}(p(K))$ in only this exposed vertex. Then l is a line which does not intersect the interior of $\text{conv}(p(K))$ and which does not contain either arc connecting v_i to v_j and so v_i, v_j form an exposed pair. ■

Define a plane P to be a *boundary plane* of K if it is vertical and does not intersect the interior of $\text{conv}(K)$. This means it is the projection preimage of a supporting line of $\text{conv}(p(K))$. We also define v_i, v_j in K to be an *edge pair* if they share an edge of $\text{conv}(K)$ and a boundary plane P which does not contain either arc connecting v_i to v_j . We next show that if the projection of our knot isn't exposed, then there is an edge pair.

Lemma 9 *If K is a knot with $p(K)$ not exposed, then there is an edge pair v_i, v_j .*

Proof: Since $p(K)$ is not exposed, Lemma 8 tells us there is an exposed pair of vertexes $p(v_i), p(v_j)$. This exposed pair shares a line l with l disjoint from the interior of $\text{conv}(p(K))$, and not containing either arc connecting $p(v_i)$ to $p(v_j)$. Looking at projection preimages, this means that there is a boundary plane $P = p^{-1}(l)$ with P containing v_i and v_j , but with P not containing either arc connecting them. As their projections are exposed, they must share a face F of $\text{conv}(K)$, and both lie on the boundary of that face.

Choose one arc around the boundary of F . This will contain some number of intermediate vertexes. If there are no such vertexes, then v_i and v_j share an edge of $\text{conv}(K)$ and we are done. Otherwise, choose an intermediate vertex v_k . Denote the arcs connecting v_i to v_j by A, B . The vertex v_k lies on one of those two arcs, and so without loss of generality, suppose it is B . Thus, $B = B_1 \cup B_2$, where B_1 is an arc connecting v_i to v_k and B_2 is an arc connecting v_k to v_j . The arc B does not lie in P so either B_1 does not lie in P or B_2 does not lie in P . If B_1 does not, then v_i and v_k are a pair of vertexes in P which both lie on a boundary arc of F but with fewer intermediate boundary vertexes. If B_2 is not contained in P , then v_k and v_j are a pair of vertexes in P which both lie on a boundary arc of F but with fewer intermediate boundary vertexes. Thus, in every case where there is an intermediate vertex on the boundary of F , we can choose new vertexes v_i and v_j in P with neither arc connecting them in P but with fewer vertexes between them. This allows us to use induction to reduce to the base case when there are

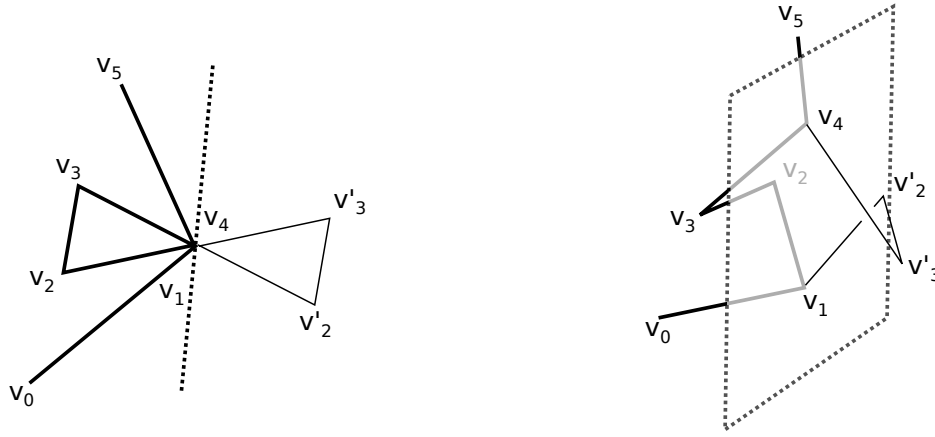


Figure 3.4: An example of a reflection of an arc across a boundary plane. The left diagram is the projection into the plane.

no intermediate vertexes and so the result holds. ■

So far we have shown that if our knot does not have an exposed projection, then there is an edge pair, and so we can reflect one arc connecting the edge pair across a common boundary plane to expand the projection. We now show that this expansion must have a limiting polygon.

Lemma 10 *If K_i is a sequence of knots with $K_{i+1} = K_i$ or $K_{i+1} = r_i(K_i)$ where r_i is a reflection of an arc connecting an edge pair across a boundary plane, then the sequence K_i converges to a limit polygon K^* .*

Proof: Since the plane of reflection P_i is vertical, it projects to $p(P_i) = l_i$. Reflection of an arc across a line which does not intersect the interior of the convex hull does not decrease the distance between pairs of points. Thus, each distance between pairs $p(v_i)$ and $p(v_j)$ is increasing, but it is also bounded above by half of the arclength of the knot. Thus, each distance between pairs of vertex projections must converge.

We now consider two cases. First suppose there is a collection of three vertexes projections, $p(v_i), p(v_j), p(v_k)$ whose pairwise distances converge to a strict triangle inequality.

Then there exists an N so that for all $n \geq N$, K_n has $p(v_i), p(v_j), p(v_k)$ satisfying a strict triangle inequality, meaning those three vertex projections are not collinear. Thus, since the location of a point in a plane can be determined by its distance to any three non-collinear points, then the position of every other vertex projection converges. Since none of the heights were changed, the location of every vertex of K_i converges and so there is a limit polygon K^* .

In the second case, every triple of vertex projections $p(v_i), p(v_j), p(v_k)$ have distances which converge to a triangle equality. This means every triple of projections converge to collinearity, since only collinear points satisfy triangle equality. Thus, taking a pair $p(v_i)$ and $p(v_j)$ and the line through them, every other vertex must converge to a specific point on that line. Thus, the location of the vertexes projections converge and the heights of the vertexes were unchanged so the location of the vertexes converge giving a limit polygon K^* . ■

We now know that a limiting polygon exists. We now use information about that limit to get information about elements of the sequence. We first show that vertexes which are exposed in the limit are actually exposed in finite time.

Lemma 11 *If K_i is a sequence of knots with $K_{i+1} = K_i$ or $K_{i+1} = r_i(K_i)$ where r_i is a reflection of an arc connecting an edge pair across a boundary plane and v_j is a vertex of the knots which has exposed projection in the limit K^* , then there exists an N with v_j having exposed projection in K_n for all $n \geq N$.*

Proof: Because $p(v_j)$ is exposed in the limit, it is a vertex of $\text{conv}(p(K^*))$ so there is a line l which separates the limit of $p(v_j)$ from the limit of all other vertex projections. This line l separates the plane into two open sets. The convergence of each point, means that for each vertex v_k there is a natural number N_k with $p(v_k)$ on the correct side of l in all K_n with $n \geq N_k$. Taking $N = \max(N_k)$, we get that for all $n \geq N$, K_n has all vertex

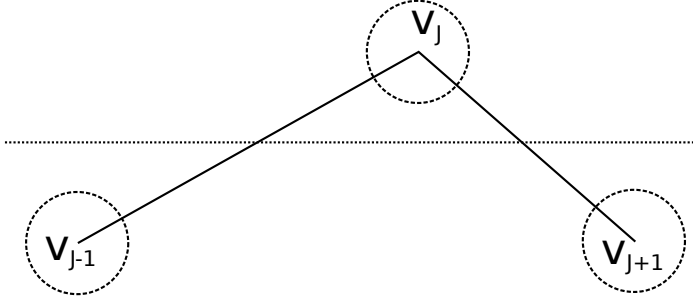


Figure 3.5: A model of a triple of points near a vertex which is exposed in the limit, along with a line separating this exposed vertex from the rest of the knot

projections on the same side of l as K^* . This means that for all K_n with $n \geq N$, there is a line separating $p(v_j)$ from all other vertexes, so $p(v_j)$ is an exposed vertex of $p(K_n)$. ■

So far we have allowed any choice of reflection of arc connecting an edge pair. We will now show that if we make a specific choice of reflection, then the limit will be exposed. We define $\mu(p(K))$ to be the sum over pairs of vertexes v_i, v_j of the distance between v_i and v_j .

Lemma 12 *Suppose K_i is a sequence of knots with $K_{i+1} = K_i$ or $K_{i+1} = r_i(K_i)$ where r_i is a reflection of an arc connecting an edge pair across a boundary plane, with K_{i+1} chosen so that the number of vertexes v_j with turning angle at $p(v_j) = \pi$ is reduced if possible, and otherwise chosen so that $\mu(p(K_{i+1}))$ is maximized. Then, the limit polygon K^* is exposed.*

Proof: Seeking a contradiction, suppose K^* has a projection which is not exposed. This means there is a reflection move on K^* . This involves increasing $\mu(p(K^*))$ by an amount δ . Taking the convex hull and the sums of distances between vertex projections are both continuous operations which means the maximum change in $\mu(p(K_i))$ must converge to a value greater than or equal to δ . Our choice of reflections, however, ensures that the maximum change in $\mu(p(K_i))$ converges to zero. This is a contradiction and so

the limit K^* must be exposed. ■

We now know that if chosen properly, then the reflection moves will have an exposed limit. We next show that the limit is reached in finite time, first by proving it when the limit is full dimensional and then again when the limit is subdimensional.

Lemma 13 *Suppose K_i is a sequence of knots with $K_{i+1} = K_i$ or $K_{i+1} = r_i(K_i)$ where r_i is a reflection of an arc connecting an edge pair across a boundary plane, with K_{i+1} chosen so that the number of vertexes v_j with turning angle at $p(v_j) = \pi$ is reduced if possible, and otherwise chosen so that $\mu(p(K_{i+1}))$ is maximized. If the projection of the limit polygon $p(K^*)$ is full dimensional, then there exists an N so that for any $n > N$, $K_{n+1} = K_n$.*

Proof: Lemma 12 tells us that the projection of the limit $p(K^*)$ is an exposed polygon. The fact that K^* is an exposed polygon tells us that $K^* = \bigcup_{l=0}^m A_l$, where A_l is an arc connecting adjacent exposed vertexes of K^* . We also know that since K^* is full dimensional, for any pair of vertexes v_{l_1}, v_{l_2} on the interior of distinct arcs A_{l_1}, A_{l_2} , the line segment connecting $p(v_{l_1}), p(v_{l_2})$ intersects the interior of the convex hull of $p(K^*)$. The continuity of taking the convex hull and taking convex combinations of vertexes tells us that there is a natural number N_{l_1, l_2} so that for every $n \geq N_{l_1, l_2}$, K_n has the line connecting v_{l_1}, v_{l_2} intersects the interior of the convex hull of $p(K_n)$. Taking N to be the maximum over this finite number of bounds, we get that for every $n \geq N$, any line connecting vertexes on distinct arcs A_{l_1}, A_{l_2} intersects the interior of the convex hull of $p(K_n)$, and so every edge pair lies in one of the arcs $\{A_l\}_{l=1}^m$.

The fact that every edge pair lies in one of the arcs $\{A_l\}_{l=1}^m$ tells us that any reflection of arc connecting an edge pair must have either the reflected arc or the stationary arc containing all vertexes which are exposed in $p(K^*)$. Without loss of generality, we can assume that the stationary arc is the one which contains all vertexes exposed in $p(K^*)$.

Thus, every vertex which is exposed in $p(K^*)$ is fixed for all $n > N$. For any vertex v_j on the interior of one of the arc A_l , we have the triple of vertexes v_j, v_{l_0}, v_{l_k} , where v_{l_0}, v_{l_k} are the endpoints of the arc A_l . The distance $d_1 = d(p(v_{l_0}), p(v_{l_k}))$ is fixed, the distances $d_2 = d(p(v_{l_0}), p(v_j))$ and $d_3 = d(p(v_j), p(v_{l_k}))$ are non-decreasing, and the limit satisfies $d_1 = d_2 + d_3$ which is the minimum for $d_2 + d_3$, so for every $n \geq N$, $d_1 = d_2 + d_3$ which uniquely determines the location of v_j . Thus, for every $n \geq N$, every vertex is fixed. Thus, $K_{n+1} = K_n$. ■

Lemma 14 *Suppose K_i is a sequence of knots with $K_{i+1} = K_i$ or $K_{i+1} = r_i(K_i)$ where r_i is a reflection of an arc connecting an edge pair across a boundary plane, with K_{i+1} chosen so that the number of vertexes v_j with turning angle at $p(v_j) = \pi$ is reduced if possible, and otherwise chosen so that $\mu(p(K_{i+1}))$ is maximized. If the projection of the limit polygon $p(K^*)$ is subdimensional, then there exists an N so that for any $n > N$, $K_{n+1} = K_n$*

Proof: Lemma 12 tells us that the projection of the limit $p(K^*)$ is an exposed polygon. There can only be finitely many r_i which reduce the number of turning angle π vertexes so there is a number M so that for every $n > M$, no such reflection is possible. The fact that $p(K^*)$ is subdimensional means that each exposed vertex $p(v_i)$ has turning angle π , so both edges coming out from $p(v_i)$ go in the same direction. By Lemma 11, there is an N with $p(v_i)$ exposed in K_n for every $n \geq N$. If $n > \max(N, M)$ and $p(K_n)$ is not subdimensional, then there are two distinct edges of $\text{conv}(p(K_n))$ coming from $p(v_i)$, so at least one l does not contain the edges coming out of $p(v_i)$. This means that there is an edge pair made of v_i and another vertex v_j with $p(v_j)$ on l . Reflecting an arc connecting v_i to v_j reduces the number of vertexes with turning angle π . This contradicts the choice of M so we know that for all $n > \max(M, N)$, $p(K_n)$ is subdimensional. Since a subdimensional polygon has exactly its endpoints as exposed vertexes, every reflection

move between subdimensional polygons changes which two vertexes are exposed, and for every $n > N$ the two exposed vertexes of $p(K^*)$ are exposed vertexes of $p(K_n)$, no reflection can be applied to K_n . Thus, for every $n > \max(N, M)$, $K_{n+1} = K_n$. ■

Theorem 15 *For any knot K , there is a finite number of reflections r_i of arcs connecting edge pairs across boundary planes, generating a sequence $K = K_0, \dots, K_n$, with $r_i(K_i) = K_{i+1}$ and $p(K_n)$ an exposed polygon.*

Proof: By Lemma 9 there is a reflection as long as the result is not yet exposed. By lemmas 13 and 14 we know that if those reflections are chosen correctly, only finitely many are required to reach the limit polygon, which by Lemma 12 is an exposed polygon. ■

3.1.2 Moving From Exposed to Convex

To reach a convex polygon, we need to make the number of unnecessary intersections of edge projections go to zero. We measure this distance from being an embedding by taking the *incidence* of the knot to be $I(K) = |\{(e_i, e_j) \text{ such that } p(e_i) \cap p(e_j) \text{ non-trivial}\}|$, where the e_i are edges of the knot. Using the the previous section we can get the following theorem about polygonal knots with thickness.

Theorem 16 *Any knot K can be transformed into a knot K' whose orthogonal projection into the $x - y$ plane is an exposed polygon using a finite number of height preserving, thickness non-decreasing reflections r_i , with $I(K') \leq I(K)$ and each r_i in the closure of the interior of moves which do not decrease thickness.*

Proof: We first take the standard orthogonal projection of K into the $x - y$ plane. This projection gives a polygonal loop, $p(K)$, with possible intersections. We can apply

Theorem 15 to find a sequence of finitely many reflections r_i of arcs connecting edge pairs across boundary planes P_i which take K to K' with $p(K')$ exposed.

Each of these reflection moves is across a plane parallel to the z -axis, and so the z coordinate is unchanged, making the process height invariant. We also are reflecting at each step across a plane which does not intersect the convex hull of the current knot, which means that by Lemma 6 the thickness is not decreased by any reflection. The fact that the reflection is of an arc connecting an edge pair means that P_i lies in a positive length interval of planes which contain the same edge pair but do not intersect the interior of the convex hull. Thus, r_i is in the closure of the interior of moves which do not decrease thickness. Finally, if we have two edges whose projections intersect non-trivially after a reflection move, then either both were fixed, both moved, or exactly one moved. If both moved or both were fixed, then the non-trivial intersection was present before the reflection. If one moved and the other didn't, then they each are placed on opposite sides of $p(P_i)$. Thus, their intersection lies on $p(P_i)$ and was fixed by r_i meaning it was present before the reflection. Therefore there can be no newly created incident edge pairs, and so $I(K') \leq I(K)$. Thus, all the properties in the theorem are shown. ■

Our next step is to find reflections which decrease the incidence of the knot projection, without increasing thickness or changing the set of minimal height vertexes. We know that we have injectivity at the vertexes of the convex hull, so we turn our attention to the edges. Whenever injectivity fails inside an edge, we will push a part of the preimage of that edge out slightly to remove some of the incidences and continue the process.

Lemma 17 *If K is a knot with $p(K)$ an exposed polygon which is not convex, there exists a reflection move or affine transformation r with $I(r(K)) < I(K)$, $r(K)$ having no fewer minimal height vertexes than K , and r in the interior of moves which do not decrease thickness.*

Proof: We first consider the special case where $p(K)$ is subdimensional. In that case, K lies in a vertical plane, so we can apply an affine transformation r moving this plane to horizontal. This means $p(r(K))$ is an embedding, so $I(r(K))$ is zero, $r(K)$ has the same thickness as K , and $r(K)$ has the maximum number of minimal height vertexes.

We next move to the case where $p(K)$ is full dimensional. Note that if $p(K)$ is an exposed polygon which is not convex, then there is an edge e of the convex hull of $p(K)$ for which $p|_{p^{-1}(e)}$ is not an injection. The set $p^{-1}(e)$ is an infinite strip, with $K \cap p^{-1}(e)$ going from one side of the strip to the other. We will denote this arc A for simplicity. The fact that A moves from one side of the strip to the other tells us that the convex hull of A separates the strip into a top and bottom portion. In particular, the doubling back means that A doesn't live inside the lower boundary of its convex hull. Thus, there is a line l defining the bottom portion of the convex hull of A and a subarc a with both ends on l but whose interior misses l . We can assert this by choosing a point α which lies directly above another, and proceeding forward and back until we reach the lower boundary of the convex hull of A at the points α_+ and α_- . The knot being injective means that the arc connecting α_- to α_+ through α separates the convex hull, and so anything on the line segment connecting α_- to α_+ would be separated from the endpoints of A . We will reflect across a plane containing l .

If we choose the plane of reflection to be perfectly vertical, then we have accomplished nothing, but if the plane of reflection is too shallow, we may create problems for thickness or minimal height vertexes. We will consider a cylindrical coordinate system, where the center of the cylinder is the line l about which we are rotating. We orient this coordinate system so the angle 0 corresponds to the half plane directly below l and the angle π to the half plane above l . The fact that l lies on the boundary of the convex hull means we can assert that the entire knot has angles in $[0, \pi]$, and the fact that l is a lower boundary of the convex hull of A means that all angles are greater than 0. The knot K is compact,

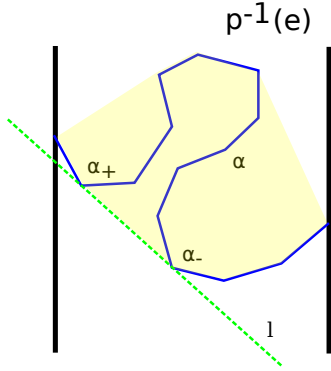


Figure 3.6: An example of $p^{-1}(e)$ with the convex hull of A highlighted

which means it attains its minimal angle θ_{min} . This means that if we choose a plane through l at angle $0 < \epsilon < \theta_{min}$, this plane intersects the convex hull of K only in the line l . In particular, Lemma 6 tells us that reflecting across this plane is a reflection move r with $r(K)$ having no lower thickness than K , as is any nearby reflection \tilde{r} , so r is in the interior of moves which do not decrease thickness. The height of each vertex after the reflection is a continuous function of the angle ϵ , and so for a sufficiently small ϵ , any vertex which was above the minimal height will stay above the minimal height, and none at the minimal height are moved, so the set of minimal height vertexes is unchanged. Finally, we seek to show that $I(r(K)) < I(K)$.

Any pair of edges which are both unmoved will have their incidences unchanged. Among those that are moved, we have at least some non-trivial intersections, by our choice of a . Further, the moved portion a is moved to a half plane h which is not vertical, and therefore $p|_h$ is injective. Thus, there are no incidences among pairs of edges where at least one is moved. Thus, $I(r(K)) < I(K)$ and so the result holds. ■

This allows us to state the theorem which moves us to the next phase of the algorithm.

Theorem 18 *For any knot K , there is a finite sequence of knots $\{K_i\}_{i=0}^n$ and reflection moves r_i satisfying the following.*

- $K_0 = K$
- $p(K_n)$ is convex
- The set of minimal height vertexes is nondecreasing as i increases.
- Each reflection move r_i is in the closure of the interior of moves which do not decrease thickness.

Proof: We induct on $I(K)$. Regardless of the value of $I(K)$, we can apply Theorem 16 and get a finite sequence which ends in an exposed polygon. If this polygon is convex, then we are done. Otherwise we apply Lemma 17, which reduces the number of incidences, and so the inductive hypotheses completes the result. ■

3.2 Flattening the Knot

In this section our goal is to produce a knot which is convex and planar using thickness non-decreasing moves. We will do so inductively using the number of vertexes at the minimum height. This will be done using two theorems.

Theorem 19 *If a knot has a convex orthogonal projection into the $x - y$ plane, but is not planar, then there is a pair of reflection moves or a rotation that will increase the number of minimum height vertexes by at least one, with a neighborhood which does not decreasing the thickness.*

Proof: There must be at least one vertex that attains the minimum height among vertexes. Consider first the case where there is exactly one vertex v which is at the minimum height. We can apply a rotation and change the minimum height vertex into a maximum height vertex. Intermediate value theorem tells us that for each other vertex,

v' , there is an intermediate rotation which makes the height of v equal the height of v' . Since there are finitely many vertexes, there is a first vertex, w for which this happens. Since this is the first vertex to pass the height of v , v must still be a minimum height vertex, and now w is also. Thus, we have increased the number of minimum height vertexes from one to at least two. As a rotation does not affect the knot thickness in any way, the result is shown in this case.

Now consider the case where there are at least two vertexes which attain the minimum height. Find a pair of such vertexes, v_1, v_n , with the property that there is an arc of the knot connecting them with no minimum height vertexes, and with at least one vertex. The fact that the knot is not planar guarantees the existence of such an arc. Since the knot is convex in the projection, there is a vertical plane with the arc in the closure of one side and the complementary arc in the closure of the other side. We will use the fact that an arc may be rotated using a pair of reflection moves through a common axis. We can then use this to rotate the arc away from the separating plane. Each of the intermediate vertexes, $\{v_i\}_2^{n-1}$ form an angle θ_i with the line connecting v_1 to v_n , oriented so 0 represents a point lying at the height of v_1 and v_n , and $\pi/2$ representing lying above the line connecting v_1 to v_n . There is a minimal such angle θ_j . Thus, if we rotate the arc connecting v_1 to v_n down by an angle θ_j , we add v_j to the set of vertexes at the height of v_1 and since $\theta_j \leq \theta_i$ for $2 \leq i \leq n-1$, no vertex can have gone below v_1 and so we have added a vertex to the set of minimum height vertexes.

Consider two points in the realization, v, w and a rotation angle θ with $0 \leq \theta \leq 2\theta_j$. We seek to apply Lemma 5 and so we would like to know that the distance between v, w is increased by the rotation, which means it suffices to show that their squared distance is increased. If both are unmoved by the rotation, or if both are rotated, then the distance between them is unchanged. Thus, we can suppose that v is moved, and w is fixed. We will consider cylindrical coordinates, with the axis of rotation the center of the cylinder.

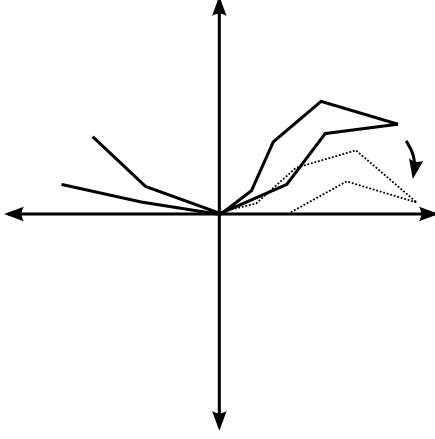


Figure 3.7: An example of a rotation which increases the number of minimum height vertexes, shown from a projection which is parallel to the axis of rotation.

This causes the height and radius of both points to be unchanged. Further, since we are rotating about an axis which includes two vertexes which are absolute minimums, we can presume that the radii are both non-negative, that the fixed point, w , has angle ϕ_w between π and $\pi/2$, and that the point being rotated, v , has angle ϕ_v which starts between $\pi/2$ and θ_j . Let ϕ be the difference between ϕ_v and ϕ_w . The height coordinates are both constant, so the difference in the squared distance reduces to the following.

$$(r_1 \sin(\phi))^2 + (r_1 \cos(\phi) - r_2)^2 = r_1^2 - 2r_1 r_2 \cos(\phi) + r_2^2$$

Because $\phi_v > \theta_j$, we know that $\phi < \pi - \theta_j$ initially. Since $\theta < 2\theta_j$ we can observe that $|\pi - \phi|$ is reduced. This means that $\cos(\phi)$ is decreased by the move, so the distance between the points is increased. This means that every rotation by an angle θ with $0 < \theta < 2\theta_j$ does not decrease thickness, so the particular rotation by θ_j has a neighborhood which does not decrease thickness. ■

We now combine theorems 16 and 19 for the following theorem.

Theorem 20 *Any knot may be made convex and planar using a sequence of finitely many moves consisting of affine transformations, reflections, or pairs of reflections, such that each move is contained in the closure of the interior of moves which will not increase the thickness.*

Proof: We do this using induction on the number of vertexes which fail to attain the minimum height. If there are no vertexes which fail to attain the minimum height then all vertexes are in a common plane. Applying Theorem 16 gives a finite sequence of moves which makes it convex, does not change the height, and is in the closure of the interior of moves which do not decrease the thickness and so we are done. Now suppose that we can achieve the desired result if there are less than n vertexes which attain the minimum height, and that K is a knot which has exactly n vertexes which fail to attain the minimum height. We can then apply Theorem 16 to get a finite sequence of j reflections which do not affect the height, are in the closure of the interior of moves which do not decrease the thickness, and give us a knot configuration K_2 which is convex in projection. Since the height is unchanged we still have n vertexes which fail to attain the minimum height. We can then use Theorem 19 to get a pair of reflections or a rotation in the closure of the interior of moves which do not decrease thickness, which will give us a knot K_3 with fewer than n minimum vertexes. Finally, we can use the inductive hypothesis to get a sequence of k moves in the closure of the interior of moves which do not decrease thickness which results in a convex planar polygon. Thus, K can be made convex and planar using $j + k + 1$ moves in the closure of the interior of moves which do not decrease thickness. Therefore, by induction, any knot can be made convex and planar using a finite sequence of moves in the closure of the interior of moves which do not decrease thickness. ■

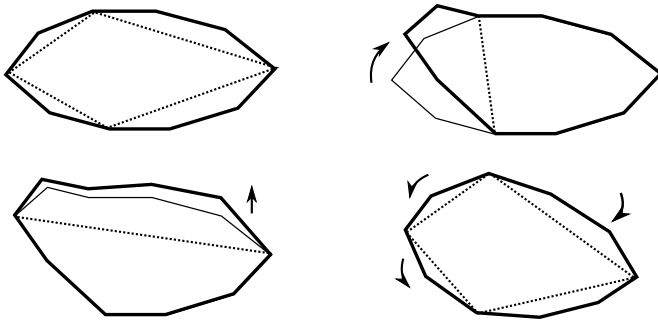


Figure 3.8: An example of applying the hextuple reflection move to a decagon. The initial diagram has the four distinguished vertexes connected by dotted lines.

3.3 Convex and Planar made Regular

3.3.1 The Move

The move will be a sequence of six reflections, but the net result can be explained much more clearly. We will take four vertexes and look at the planar knot as being the quadrilateral joined directly by those four vertexes, along with up to four flaps.

The result of the move is equivalent to allowing only the distinguished four vertexes to pivot in the plane, and then pushing two opposite vertexes together, allowing the complementary two to spread apart. This causes two interior angles to shrink and two interior angles to grow. We will pick two vertexes whose interior angles are large and two whose interior angles are small so applying this move minimally will make one of the four regular.

Informally, the way we achieve this type of move using reflections is that we reflect through a plane containing two of the flexible vertexes to bring the complementary vertexes closer together, and then use a reflection through the pair we moved to make the four planar. Finally we use up to four more reflections to bring the four flaps back into the common plane.

3.3.2 Picking Vertices

As mentioned above, we find a collection of four vertexes, two which have large interior angle and two which have small interior angle, in an alternating pattern around the knot.

Lemma 21 *For any convex non-regular polygon in the plane, there exists an ordered set of four vertexes, v_1, w_1, v_2, w_2 with the interior angle of v_i smaller than regular, and the interior angle of w_i larger than regular.*

Proof: For this, we first note that if the polygon is not regular, then it must have a vertex, w_1 , with an interior angle which is too big and a vertex, v_1 , whose interior angle is too small, since the sum of the angles is fixed. Without loss of generality, choose v_1 and w_1 to be separated only by vertexes with regular angles in at least one of the arcs. Next, we consider the arc consisting of just the two edges connected to w_1 . This arc has longer end to end distance than if the polygon was regular. This means that the complementary arc must also have longer end to end distance. Since we are dealing with a convex polygon, the end to end distance is an increasing function of the interior angles, and so there must be some second vertex w_2 which has an interior angle which is too large. This vertex cannot be between v_1 and w_1 so without loss of generality, choose it to be the closest such vertex to v_1 on the other side from w_1 . Thus, the arc connecting w_1 to w_2 through v_1 consists only of vertexes with angles which are regular or smaller than regular. This means that this arc has shorter end-to-end distance than in the regular polygon, so the complementary arc has shorter end-to-end distance than the regular polygon, meaning it must also have a vertex, v_2 , which has an angle which is smaller than regular. Thus, we have a sequence of ordered vertexes v_1, w_1, v_2, w_2 , with v_1, v_2 having angles which are smaller than regular and with w_1, w_2 having angles which are bigger than regular. ■

3.3.3 Choosing Reflections

We will assume the knot lies in the $x - y$ plane and form a transformation of the knot T , consisting of up to six reflections which result in $T(K)$ being planar and having more regular vertexes than K . The first reflection will reflect the arc connecting w_1 to w_2 through v_1 across a plane which makes an angle of θ to the $x - y$ plane. There are generally two such choices so we will choose the one which puts the vertex v_1 to a non-negative z coordinate. The second will reflect the arc connecting v_1 to v_2 through w_2 , and will be chosen in such a way as to make the four vertexes v_1, v_2, w_1, w_2 coplanar. There are generally two such choices so choose the one which maximizes the z coordinate of w_2 . Finally, the four arcs connecting the vertexes of our highlighted quadrilateral may be out of alignment, so we will reflect them each across a plane which will bring them into the common plane of v_1, v_2, w_1, w_2 . Again there are two such choices so we will choose the one which moves each flap the shortest distance. This gives a family of transformations, T_θ , for each real number, θ between 0 and $\pi/2$, with $T_\theta(K)$ continuous in θ . This leads us to the next result.

Theorem 22 *Any convex planar knot can be made regular using a sequence of finitely many moves, each move consisting of at most six reflections, with each such move in the interior of moves which do not decrease thickness.*

Proof: We will show that there is a choice of θ for which $T_\theta(K)$ has exactly one of the four vertexes have a regular interior angle without switching any of the other four between larger than regular interior angle and smaller than regular interior angle. For this, we consider the vectors $e_1 = w_1 - v_1$, $e_2 = v_2 - w_1$, $e_3 = w_2 - v_2$, and $e_4 = v_2 - w_1$. These are the four edges of the inscribed quadrilateral formed by those four vertexes. We then look at the function $f(K) = (e_1 \times e_2) \cdot (e_3 \times e_4)$. For $\theta = 0$, $f(T_\theta(K)) > 0$. For $\theta = \pi/2$, $f(T_\theta(K)) < 0$. Thus, since f is a continuous function and T_θ is a continuous

function of θ , we use the intermediate value theorem to observe that there is a choice θ_0 for which $f(T_{\theta_0}(K)) = 0$, so $e_1 \times e_2$ and $e_3 \times e_4$ are perpendicular vectors.. The configuration $T_{\theta}(K)$ is always planar, so the vectors $e_1 \times e_2$ and $e_3 \times e_4$ are parallel. This means that the two vectors are both parallel and perpendicular, which can only be the case if one of them is the zero vector. Thus, either $e_1 \times e_2$ is zero or $e_3 \times e_4$ is zero, so in $T_{\theta_0}(K)$, one of the v_i is collinear with w_1 and w_2 .

For the remainder of the proof $\theta \leq \theta_0$. This means that in particular $T_{\theta}(K)$ is still an embedding. Thus, we have a well defined notion of the sign of a turning angle, where the sign of all turning angles in $T_0(K)$ are positive. The fact that the interior angle of v_i in $T_0(K)$ is smaller than regular, the turning angle at v_i in $T_0(K)$ is larger than regular. Because v_i is collinear with w_1 and w_2 in $T_{\theta_0}(K)$, the turning angle of v_i in $T_{\theta_0}(K)$ is negative. This means that by the intermediate value theorem, there exists an angle θ_1 with the turning angle of v_i in $T_{\theta_1}(K)$ regular.

There may be multiple choices of θ with $T_{\theta}(K)$ having a greater number of regular angles than K . We then choose the smallest θ which makes at least one of the four changing angles regular. Thus, one particular angle is made regular, and the remainder stay on the same side of regular, either staying larger than regular or staying smaller than regular. We note that from corollary 4, the long range thickness need not be considered. One possibility is that the smallest angle is unchanged, which means that for any T in a neighborhood of T_{θ} , the thickness of $T(K)$ is the same as the thickness of K . The other possibility is that the smallest angle is one of the v_i and so is larger, meaning that $T_{\theta}(K)$ is thicker than K and so since thickness is continuous, a neighborhood of T_{θ} does not decrease thickness. Therefore we have increased the number of regular vertexes using a move on the interior of moves which do not decrease thickness. Applying this up to n times, where n is the number of vertexes, we can guarantee that the end result has at least n regular vertexes, and so is the regular planar polygon. ■

3.4 Result

Theorem 23 *Any equilateral polygonal knot can be made into a regular convex planar polygon using a finite number moves, consisting only of rigid motions, or up to six reflections, with each move in the closure of the interior of moves which do not decrease thickness.*

Proof: This is a simple combination of the above theorems. First, Theorem 20 shows that a finite number of such moves can make any equilateral polygonal knot planar and convex, and then Theorem 22 allows another finite number of such moves to make any equilateral polygonal planar and convex knot regular. This gives us the desired result. ■

Chapter 4

Monte-Carlo Markov Chains

In this section, we will prove that we can build an ergodic Markov chain for sampling the space of equilateral knots with thickness. The above algorithm will be necessary in showing ergodicity.

4.1 The Markov Chain

The general definition of a Markov chain is a sequence in a state space X where each entry in the sequence of states is independent of every state before the immediate predecessor. We will refer to our Markov chain as Φ . Our Markov chain is given by a set of states X in \mathbb{R}^n , a noise parameter W which is an open subset of \mathbb{R}^p with a probability measure μ_W , and a function $F : X \times W \rightarrow X$. The space of states will be $X = \text{Equ}(n, t)$. The noise parameter W will be a product of reflection moves. The space of reflection moves R is of the form (x, v_1, v_2, θ) , where x is a real number in $(0, 1)$ used to determine if we check the thickness, v_1, v_2 are a random pair of vertexes, and θ is an angle. While this R isn't clearly an open subset of \mathbb{R}^p , it can be modeled in that way by choosing the continuous variables from a rectangle, and selecting the discrete variables by using a

disjoint collection of rectangles. Thus, we use

$$R = \bigcup_{0 \leq i < j \leq n} [0, 2\pi] \times [2(n * i + j), 2(n * i + j) + 1]$$

where n is the number of edges. This space R is a disjoint collection of rectangles. The y coordinate is an angle. The width of each rectangle is 1. Which rectangle a point is in determines the i, j which represents a pair of distinct vertexes. The complete noise space is $W = R^N$, where N is a cap on how many reflections we are allowed between checking the thickness. We require that $N \geq 6$ so that we may use Theorem 23. The probability measure on W is just a multiple of the Lebesgue measure on this bounded space, which means that it has a constant probability distribution γ_W which is supported on all of W and is lower semi-continuous since W is open.

The function F in our Markov chain Φ will be defined as follows. We have a collection of N probabilities p_k which represent the probability of applying the k^{th} reflection if we already applied the $k - 1^{st}$ reflection. Given a $w \in W = R^N$ we find a sequence of variables $a_k = x_k - \lfloor x_k \rfloor$, where x_k is the x coordinate of $W_k \cong R$. These a_k live in $(0, 1)$. We find m which is one less than the first k with $a_k > p_k$, or $m = N$ if no such k exists. This m is how many reflections we will apply. When we apply a reflection to a knot $K \in \text{Equ}(n, t)$, we reflect the arc connecting the vertexes v_i and v_j across a plane determined by the angle θ , where i, j are indicated by which component of $W_k \cong R$ we are in and $\theta = y_k$ from $W_k \cong R$. Thus, we get a reflection move r_k for each k . This lets us define $F(K, w) = r_m r_{m-1} \dots r_1(K)$ if $r_m r_{m-1} \dots r_1(K) \in \text{Equ}(n, t)$ and K otherwise. This means F is a piecewise function with two pieces, one is the identity and the other is smooth.

4.2 Forward Accessible

We will use $A_+^n(x) \subseteq X$ to denote the set of states y for which there is a sequence of exactly n moves on the interior of a smooth section starting at x and ending at y . We will also define $A_+(x) = \bigcup_{n=1}^{\infty} A_+^n(x)$. One useful property a Markov chain can have is forward accessibility. A Markov chain is forward accessible if $A_+(x)$ is a set with non-empty interior, for every value of x . When the motion of the Markov chain is smooth, then the set $A_+^n(x)$ reduces to simply points reachable in n steps, but since our function is merely piecewise smooth we need the more general definition. We will prove our Markov chain is forward accessible. This will be a direct continuation of the conclusion of the previous chapter.

Lemma 24 *For every knot K , there is a finite sequence of moves m_i , $0 \leq i < N$ giving a finite sequence of knots K_i , such that $K_0 = K$, K_N is the regular planar polygon, and each m_i has a neighborhood of moves M_i , with $m(K_i) \in \text{Equ}(n, t)$ for every $m \in M_i$.*

Proof: By Theorem 23, there is a sequence of N_1 moves m_i^1 with $K_0^1 = K$, $K_{N_1}^1$ the regular planar polygon, and each move m_i^1 in the closure of the interior of moves which do not decrease thickness. This means that for any open neighborhood of the regular planar polygon, such as $\text{int}(\text{Equ}(n, t))$, there is a sequence of N_1 moves m_i^2 with $K_0^2 = K$, $K_{N_1}^2$ in the open set $\text{int}(\text{Equ}(n, t))$, and each m_i^2 on the interior of moves which do not decrease thickness, and so in particular has a neighborhood of moves M_i^2 with $m(K_i) \in \text{Equ}(n, t)$ for every $m \in M_i^2$. We also can use the same theorem to generate a sequence of N_2 moves m_i^3 with $K_0^3 = K_{N_1}^2$, $K_{N_2}^3$ the regular planar polygon and each move m_i^3 not decreasing thickness. Since each K^3 is on the interior of $\text{Equ}(n, t)$, there is a neighborhood M_i^3 of each m_i^3 with $m(K_i^3) \in \text{Equ}(n, t)$ for every $m \in M_i^3$. Concatenating these two sequences of moves, we get the desired result. ■

Theorem 25 *The Markov chain Φ is forward accessible with $\text{int}(\text{Equ}(n, t)) \subseteq A_+(K)$ for every knot K in $\text{Equ}(n, t)$.*

Proof: Let $K \in \text{Equ}(n, t)$ and $K' \in \text{int}(\text{Equ}(n, t))$. Then $K' \in \text{Equ}(n, t')$ where $t' > t$. By Lemma 24, there is a sequence of N_1 moves m_i^1 with $K_0^1 = K$, $K_{N_1}^1$ the regular planar polygon, and each m_i^1 in an open neighborhood M_i^1 with $m(K_i) \in \text{Equ}(n, t)$ for all $m \in M_i$. By the same lemma there is also a sequence of N_2 moves m_i^2 with $K_0^2 = K'$, $K_{N_2}^2$ the regular planar polygon, and each K_i^2 in $\text{Equ}(n, t') \subseteq \text{int}(\text{Equ}(n, t))$. Each reflection move can be repeated on the image knot, which means that each move m_i^2 has an inverse move $m_i^3 := (m^2)_{N_2-i}^{-1}$. Thus, K_0^3 is the regular planar polygon, $K_{N_2}^3 = K'$, and each K_i^3 is in $\text{int}(\text{Equ}(n, t))$. Since each m_i^3 has an image in the interior of $\text{Equ}(n, t)$, there is a neighborhood of each, M_i^3 with $m(K_i^3)$ in $\text{Equ}(n, t)$ for every $m \in M_i^3$. Concatenating these two sequences of moves gives a sequence of N moves m_i^4 with $K_0^4 = K$, $K_N^4 = K'$, and each move m_i^4 having a neighborhood of moves M_i^4 with $m(\hat{K}_i) \in \text{Equ}(n, t)$ for all $m \in M_i^4$. This tells us that the sequence of moves m_i^4 is on the interior of a smooth section, and so its image K' is in $A_+(K)$. ■

4.3 T-Chains

A very useful property for a Markov chain to have is being a T -chain. The precise definition requires a couple of preliminaries, but we will define it precisely in this section. To motivate it, a T -chain has moves of the Markov chain respecting the topology of the state space. We first define the *transition probabilities* $P^n(x, S)$ which is the probability of starting in x , and ending in S after n steps. These are examples of *transition kernels* which are functions $\kappa : X \times \mathcal{B}(X) \rightarrow [0, 1]$ with $\mathcal{B}(X)$ the Borel sets. A transition kernel κ is *stochastic* if $\kappa(x, X) = 1$ for all $x \in X$ and is *substochastic* if $\kappa(x, X) \leq 1$ for all $x \in X$. This allows us to note that $P^n(x, X)$ is the probability of staying in the total state space

after n steps, and so these standard probability transition functions are stochastic. From the standard transition probability and a sampling on the natural numbers $a : \mathbb{N} \rightarrow [0, 1]$, we can build the stochastic transition kernel $K_a(x, S) := \sum_{n=0}^{\infty} P^n(x, S)a(n)$.

This finally allows us to define a *T-chain* as a Markov chain for which there is a substochastic transition kernel T and a sampling distribution a with $K_a(x, S) \geq T(x, S)$, $T(\cdot, S)$ lower semicontinuous, and $T(x, X) > 0$ for every x . The lower semicontinuity is what lets us refer to T as the continuous piece of K_a , while $T(x, X) > 0$ for every x tells us that there is a significant continuous piece of K_a . With these we utilize Propositions 7.1.5 and 6.2.4 from Meyn and Tweedie's book[17].

Theorem 26 *Any Markov chain which is forward accessible and has a noise space W with a lower semi continuous probability density function γ_W , then for each x in the state space X , there is a sampling distribution $a_x : \mathbb{N} \rightarrow [0, 1]$ and a transition kernel T_x with $T_x(x, X) \neq 0$, $T_x(x, \cdot) \leq K_{a_x}(x, \cdot)$ and $T_x(\cdot, S)$ lower semi-continuous for every S .*

This theorem amounts to taking a neighborhood of the smooth path that starts at x and ends in an open set, and using the implicit function theorem to pull that information back into a neighborhood of x .

Theorem 27 *Suppose a Markov chain whose state space X is a subset of \mathbb{R}^n and has for every $x \in X$, there is a transition kernel T_x and sampling distribution $a_x : \mathbb{N} \rightarrow [0, 1]$ with $T_x(x, X) \neq 0$, $T_x(x, \cdot) \leq K_{a_x}(x, \cdot)$ and $T_x(\cdot, S)$ lower semi-continuous for every S . Then the Markov chain is a T-chain*

Proof: For each $x \in X$ there is a transition kernel T_x given by the hypothesis of the theorem. These kernels have sets $O_x = \{y \in X | T_x(y, X) > 0\}$ which are open since $T_x(\cdot, X)$ is lower semi-continuous. By assumption, $x \in O_x$ so $\{O_x\}_{x \in X}$ forms an open cover. By Lindelöf's theorem, this open cover has a countable subcover $\{O_i\}_{i \in \mathbb{N}}$.

This countable subcover corresponds to a countable set of states $\{x_i\}_{i \in \mathbb{N}}$ with corresponding transition kernels T_i and sampling distributions a_i . Let $T = \sum_{i \in \mathbb{N}} 2^{-i} T_i$ and $a = \sum_{i \in \mathbb{N}} 2^{-i} a_i$. This tells us the following.

$$\begin{aligned}
 T &= \sum_{i \in \mathbb{N}} 2^{-i} T_i \\
 &\leq \sum_{i \in \mathbb{N}} 2^{-i} K_{a_i} \\
 &= \sum_{i \in \mathbb{N}} 2^{-i} \sum_{j \in \mathbb{N}} a_i(j) P^j \\
 &= \sum_{j \in \mathbb{N}} P^j \sum_{i \in \mathbb{N}} 2^{-i} a_i(j) \\
 &= \sum_{j \in \mathbb{N}} P^j a(j) = K_a
 \end{aligned}$$

Further, $T(x, X) > 0$ for every x since the O_i form an open cover and $T(\cdot, S)$ is lower semi-continuous since each T_i is lower semi-continuous and the series converges uniformly. ■

We can combine these two results to get the following.

Corollary 28 *The Markov chain Φ is a T -chain.*

Proof: By Theorem 26 and Theorem 27, Φ is a T -chain since it is forward accessible and has a density function which is supported and constant on an open set, and so in particular is lower semi-continuous. ■

A sequence of probability distributions μ_k is *tight* if for every $\epsilon > 0$, there is a compact set C with $\liminf(\mu_k(C)) > 1 - \epsilon$.

Lemma 29 *Any sequence of probability distributions on a compact space is tight.*

Proof: Let μ_k be a sequence of probability distributions on a compact space C . Since they are probability distributions, $\mu_k(C) = 1$ which means that $\liminf(\mu_k(C)) = 1 > 1 - \epsilon$ for every $\epsilon > 0$. ■

A Markov chain is *bounded in probability on average* if the sequence $\overline{P}_k(x, \cdot) := \frac{1}{k} \sum_{n=1}^k P^n(x, \cdot)$ is tight.

Corollary 30 *The Markov Chain Φ has a compact state space, and so is bounded in probability on average.*

4.4 Positive Harris Recurrent

We can talk about the number of times a Markov chain lies in a particular set of states as $\eta(\{x_i\}_{i=0}^\infty, S) = |\{i | x_i \in S\}|$. This allows us to define Harris recurrent. A Markov chain Φ is Harris recurrent if every set S with positive Borel measure has $P(\eta(\Phi, S) = \infty) = 1$. A Markov chain is positive if there is a probability measure on the state space X which is invariant under iteration by the Markov process. Both of these properties are extremely useful, and a Markov chain which satisfies both is called positive Harris recurrent.

A state x^* is reachable if $\sum_{n=0}^\infty P^n(x, O) > 0$ for every open set O containing x^* . We note that the regular polygon is reachable using Theorem 23. We again can utilize the book by Meyn and Tweedie by quoting proposition 18.3.2[17].

Theorem 31 *Suppose that Φ is a T -chain with a reachable state. Then Φ is positive Harris if and only if it is bounded in probability on average.*

This tells us that our Markov chain Φ is positive Harris recurrent.

4.5 Ergodic

We seek to finish by using the main theorem from Meyn and Tweedies book[17].

Theorem 32 (Aperiodic Ergodic Theorem) *Suppose that Φ is an aperiodic Harris recurrent chain, with invariant measure π . Then Φ being positive Harris recurrent is equivalent to the following.*

For every initial condition $x \in X$,

$$\sup_{S \in B(X)} |P^n(x, S) - \pi(S)| \rightarrow 0$$

as $n \rightarrow \infty$, and moreover for any two regular initial distributions λ, μ ,

$$\sum_{n=1}^{\infty} \int \int \lambda(dx) \mu(dy) \sup_{S \in B(X)} |P^n(x, S) - P^n(y, S)| < \infty.$$

We have already shown that Φ is a positive Harris recurrent T-chain, so the aperiodic ergodic theorem shows that if the chain is aperiodic then it is ergodic. A chain is aperiodic if there is no period greater than one. A chain is periodic with period d if there is a collection of disjoint closed sets $\{C_i\}_{i \in \mathbb{Z}_d}$ with the probability of going from C_i to C_{i+1} in exactly one step is one.

Theorem 33 *The Markov chain Φ is aperiodic and therefore ergodic*

Proof: Note that if the pair of points through which a potential reflection will take place is chosen to be distance exactly two from each other, then there is a choice of plane which contains the length two arc connecting them. This means that there is a choice of noise parameter which leaves the equilateral knot fixed. Thus, for any set C , there is a move which takes a state in C to itself. Suppose C_i and C_{i+1} are disjoint non-empty closed sets. Then for each x in C_i there is a move m which fixes x and so takes x to $m(x) \in X \setminus C_{i+1}$. This complement is an open set and $m(x)$ is a continuous function of m so there is a positive probability of going from C_i to $X \setminus C_{i+1}$. This ensures that no collection of multiple disjoint sets can satisfy the periodicity condition. This shows

aperiodicity which then allows us to apply the aperiodic ergodicity theorem to conclude that the Markov chain is ergodic. ■

Chapter 5

Analyzing the Data

One important aspect of any random sampling algorithm is the ability to analyze the data it provides. Throughout, we will be comparing to the *standard reflection algorithm* which is the same as our algorithm except we wait until the very end of the generation process before checking the thickness. We will analyze three aspects of the data. First, in order to help motivate the usefulness of this algorithm over previous algorithms, we will be looking at the expected number of reflection moves required to generate knots of a fixed thickness using the standard reflection algorithm and compare that to the expected number for our algorithm. The second thing we will look at is the radius of gyration, a measure of how spread out a knot is, and analyze how much of an effect thickness has on radius of gyration. Finally, we will look at the way that knot type is affected by thickness.

5.1 Expected Number of Reflections

We can compute the expected number of reflections required to generate each sample of a knot with a thickness constraint using the standard naive reflection algorithm and for the algorithm in this thesis, and compare. We need to have a cut off for how many reflections are required before the result is sufficiently independent of the starting posi-

tion, and so for the purposes of this thesis we will be applying n^2 reflections, where n is the number of edges. Thus, if p_t is the probability of a randomly generated knot having thickness greater than or equal to t , then the expected number of reflections is n^2/p_t as this is the unique solution to $x = n^2p_t + (n^2 + x)(1 - p_t)$. We can also note that the expected number of times we need to check the thickness of a knot is $1/p_t$. This means it is important to get a sense of how p_t behaves as a function of t . Using figure 5.1 we can see that p_t rapidly decreases to an asymptote of zero. We also can observe that p_t and p_{n*t} , the corresponding probability for injectivity radius, are decreasing functions of the edge length.

We will specifically look at the expected number of reflections and expected number of thickness checks for generating dodecagons. We want to compare the standard reflection algorithm, where we do all 144 reflections before checking the thickness, versus an implementation of this algorithm where we check the thickness constraint for 24 blocks of 6 reflections each. If p_t is the probability of the thickness being greater than or equal to t after 144 reflections, and q_t is the probability after only 6 reflections, then we can see the expected number of reflections are $144/p_t$ and $24 \cdot (6/q_t)$, while the expected number of checks of the thickness are $1/p_t$ and $24/q_t$. These quantities quickly grow as both p_t and q_t will rapidly approach zero, so we have graphed in figure 5.2 each quantity on a logarithmic scale. We see that the method of hexagonal reflections presented in this paper will require fewer expected reflections at any positive thickness, and for sufficiently large thicknesses, even the expected number of checks of the thickness is less. This implies that for sufficiently large thicknesses the hexagonal method is faster, and for lower thicknesses it is faster if the savings in time doing reflections is greater than the cost in time doing thickness checks.

5.2 Radius of Gyration

The *radius of gyration* is standard deviation of vertexes. This is the standard measure how spread out a knot is. One thing that should be true, intuitively, is that adding a thickness constraint will remove tightly bound knots, and so should increase the expected radius of gyration. In figure 5.3, we see that as the thickness constraint is increased, the radius of gyration increases asymptotically towards the radius of gyration for the regular planar polygon. Note that in order to make the values for the three different edge counts more comparable, we divided the radius of gyration by the number of edges, as this corresponds to rescaling so all vertex counts have the same total arclength.

Having gathered some information about the way radius of gyration responds to changes in thickness, we turn our attention to the response of the radius of gyration to changes in number of edges. It is known that when thickness is ignored, the expected radius of gyration is approximately proportional to the square root of the number of edges[18]. If we suppose that when we introduce a thickness constraint, the expected radius of gyration satisfies $\text{rgn} \approx Cn^k$, where rgn is the expected radius of gyration and n is the number of edges, then $\log(\text{rgn})$ should be approximately linear in $\log(n)$. We graphed these quantities in figure 5.4 using four thickness constraints applied to hexagons, octagons, and decagons. The slopes of these lines correspond to the growth exponent for expected radius of gyration, which is known to be $1/2$ when the thickness constraint is zero. While these approximations will be less effective at smaller numbers of edges, it can still be very useful to look at these values even at low edge counts. Calculating the secant slopes of these four curves we get the following approximations of the growth exponents.

0: .430 and .444

.025: .676 and .763

.05: .818 and .939

.075: .891 and .959

The range comes from the increase in slope in comparing octagons to hexagons, versus comparing decagons to octagons. One important piece of information we can gather from this is that even with a thickness of .025 which is less than one sixth of the maximum, the growth exponent is significantly larger than the case when thickness is ignored. We can also observe that for all thickness constraints, the approximated growth exponent increases, which mirrors the case when thickness is ignored.

5.3 Knot Types

Another important aspect of analyzing knots with a thickness constraint, is looking at the prevalence of knot types. For the small edge length knots we analyzed, the unknot is the only knot with a moderate likelihood, even for thickness free when they were least common. Even with that, however, we are still able to note that the probability of a random knot being unknotted grows quickly to one as the thickness constraint is increased.

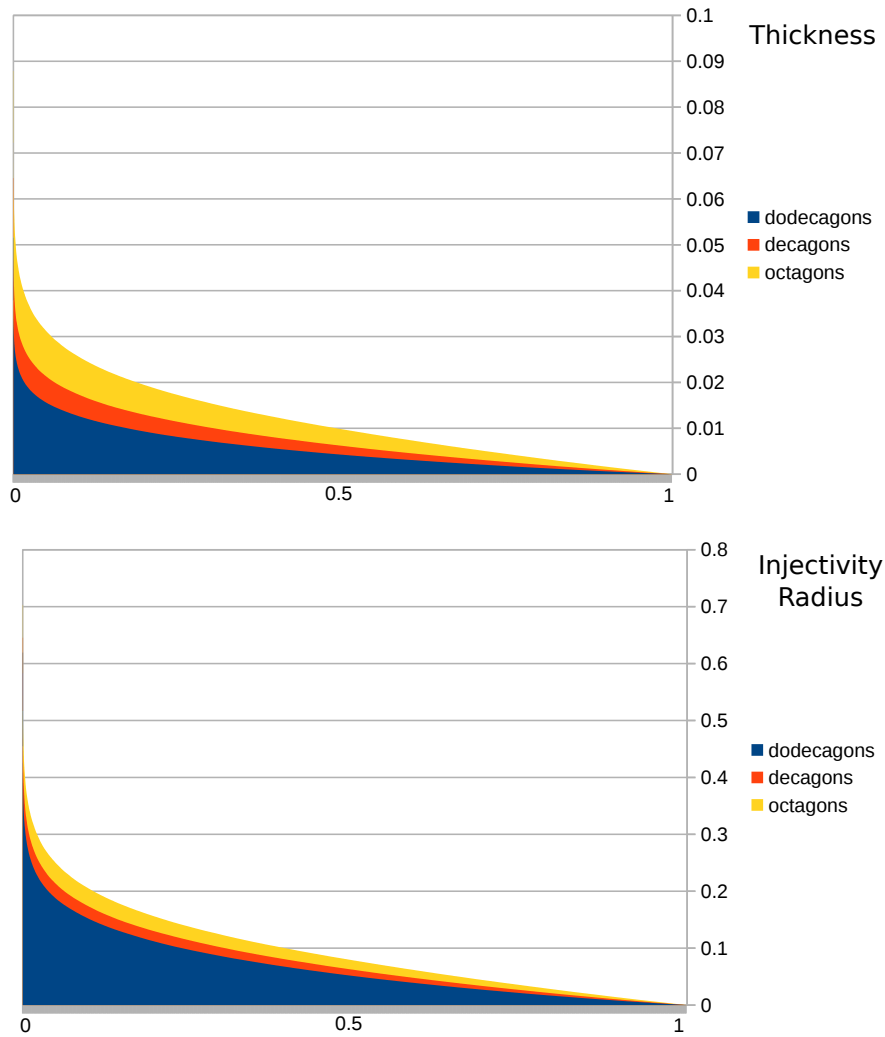


Figure 5.1: These graphs show the thicknesses and injectivity radii which correspond to various probabilities using random sample of 250000 knots of each edge length.

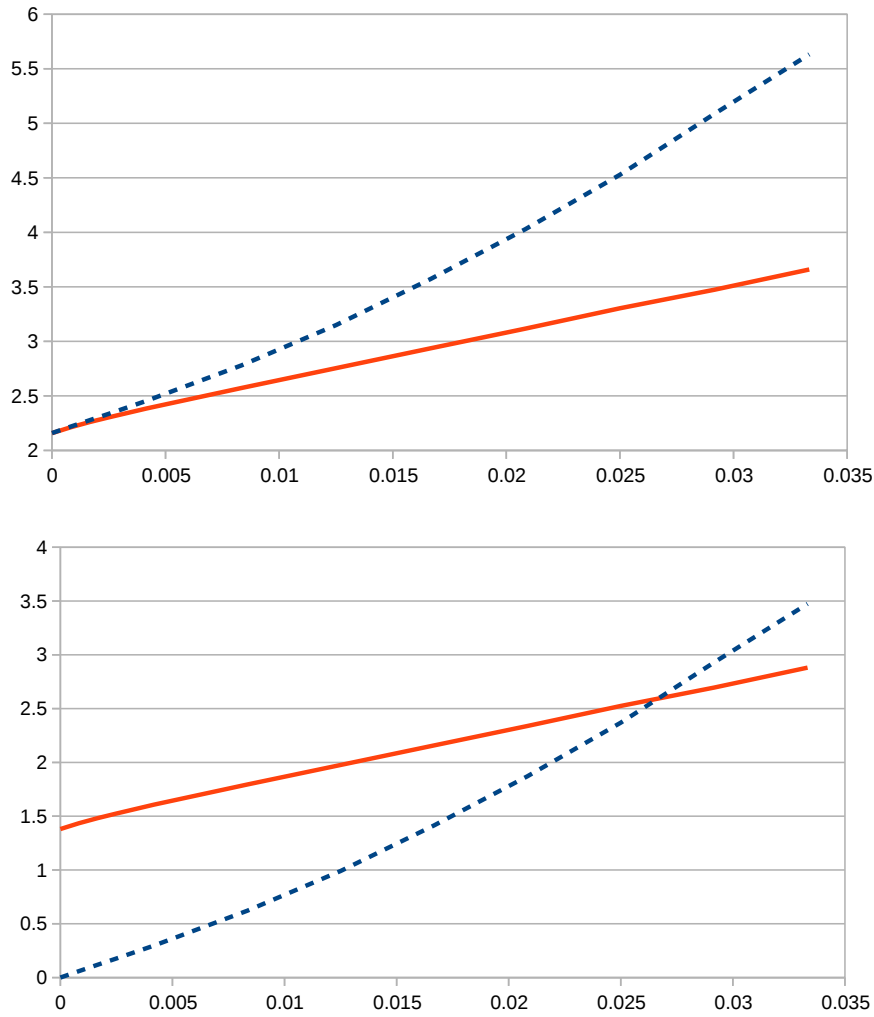


Figure 5.2: The expected number of reflections and checks of the thickness in do-decagons, respectively, graphed on a logarithmic scale against the corresponding thickness. The dashed blue line represents checking only at the end of the generation, while the solid red line represents checking every six reflections.

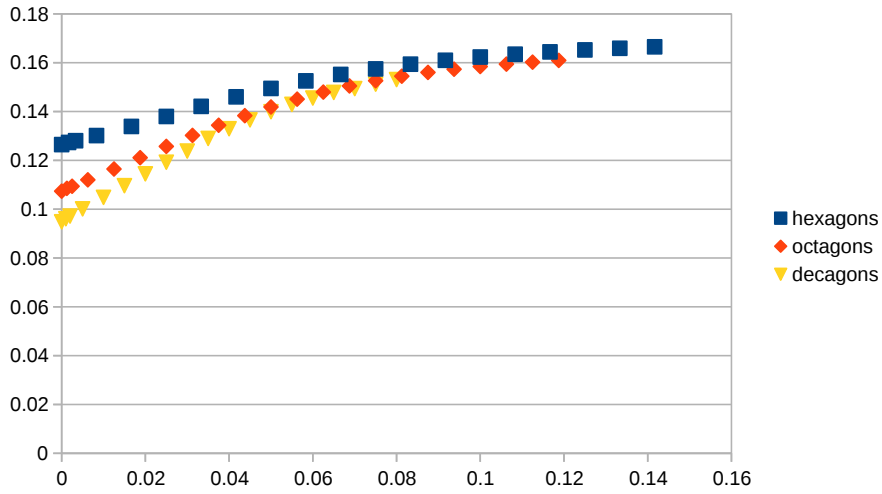


Figure 5.3: A graph showing the Radius of Gyration divided by number of edges plotted against thickness

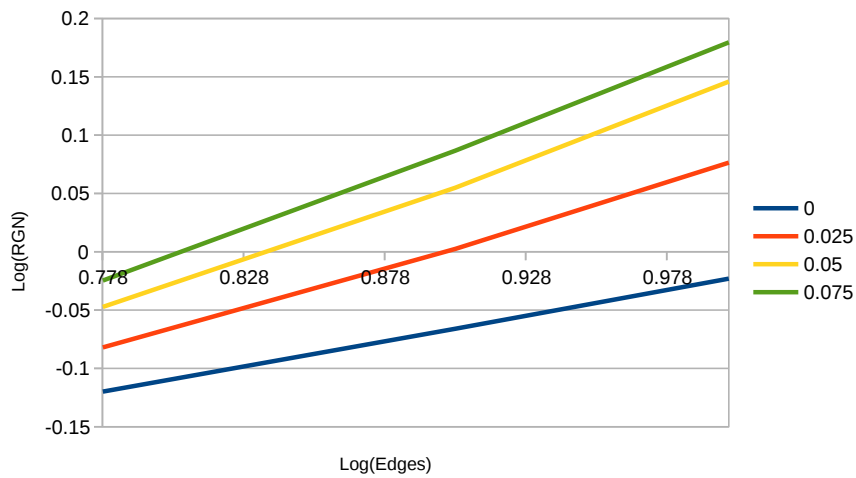


Figure 5.4: A graph for the theoretically linear graphs of the logarithm of the expected radius of gyration against the logarithm of the number of edges, using hexagons, octagons and decagons at four possible thickness constraints.

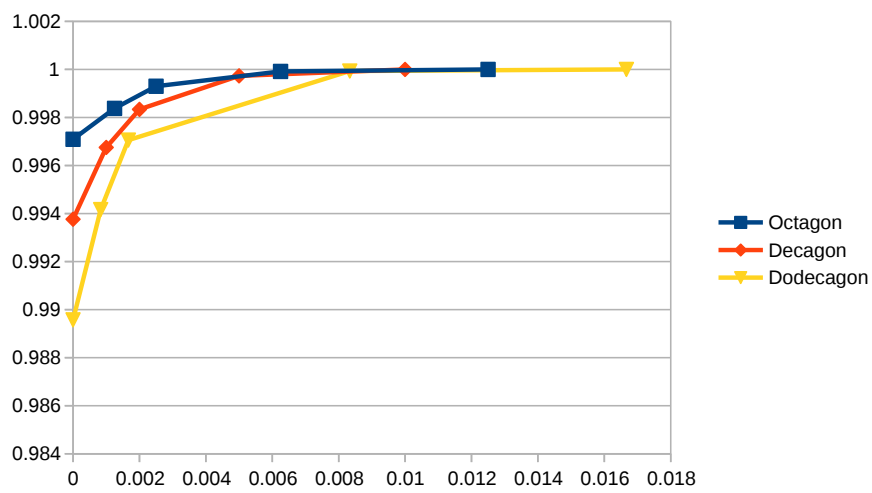


Figure 5.5: The likelihood of unknots in various polygons at different thicknesses.

Chapter 6

Conclusion and Future Work

The reflection algorithm with the use of intermediate checks that we have presented here provides a greatly expanded means of analyzing knots with a thickness. This algorithm is shown to be significantly faster for sufficiently large thicknesses. Further, the proof that this method is ergodic for every positive thickness ensures that it can be used to analyze every possible feature of geometric knots and get accurate probability distributions. With this algorithm, we have observed a number of facts about small equilateral knots with thickness. We were able to verify that the addition of thickness constraints, even small ones, results in greatly increased radius of gyration and heavily reduces the probability of knotting. Additionally, the increase in radius of gyration is greater for larger edge lengths, as indicated by the increase in growth exponent.

The next key steps are to expand this analysis to larger knots. For DNA analysis, the edge lengths need to be at least 50, and the injectivity radius should be about .1, giving a thickness of only .002. Being able to apply these methods to those ranges could give insight into applications, particularly allowing us to determine how the thickness affects knotting. The preliminary analysis here is a positive indication of that.

The other key piece of importance, is to be able to expand the knowledge about the probability distribution given by this algorithm in comparison to other algorithms, and the speed of convergence. It is unclear if the increased checks slow the mixing process of

the algorithm and so would require a greater number of successful reflections to properly mix the space. It is also unclear if the limiting probability distribution given by this algorithm exactly matches the distribution for the binning algorithm, as the probability of going between pairs of knots is altered by the intermediate checks. Finally, no prior work has shown rigorously that any method, other than generation from symplectic geometry, gives the correct probability distribution for knots. There has been much work in showing that the distributions of many functions are correct, such as radius of gyration, but this does not ensure the limiting distribution is perfectly correct. Thus, theoretical analysis of the fixed probability distribution given by this and other algorithms would go a great distance in ensuring that the methods here and in other papers are valid for applications.

Regardless of these difficulties, this algorithm clearly provides an important tool to gain some insight into the effects of thickness, and it is now only a matter of seeing how much more insight we can reasonably gather from it.

Bibliography

- [1] T. McLeish, *A tangled tale of topological fluids*, *Physics Today* **61** (2008), no. 8 40–45.
- [2] M. Doi and S. F. Edwards, *The Theory of Polymer Dynamics*. Claredon Press, 1986.
- [3] W. Fiers and R. L. Sinsheimer, *The structure of the dna of bacteriophage phi x174. iii. ultracentrifugal evidence for a ring structure*, *Journa of Molecular Biology* **5** (1962) 424–434.
- [4] J. J. Champoux, *Dna topoisomerases: structure, function and mechanism*, *Annual Review of Biochemistry* **70** (2001) 369–413.
- [5] L. F. Liu, R. E. Depew, and J. C. Wang, *Knotted single strand dna formed by treatment with escherichia coli w protein*, *Journal of Molecular Biology* **106** (1976), no. 2 439–452.
- [6] K. Millett, *Knotted regular polygons in 3-space*, *Journal of Knot Theory and its Ramifications* **3** (1994), no. 3 263–278.
- [7] R. Randell, *Conformation spaces of molecular rings*, *Physical and Theoretical Chemistry* **54** (1988) 125–140.
- [8] R. Randell, *A molecular conformation space*, *Physical and Theoretical Chemistry* **54** (1988) 125–140.
- [9] S. Wasserman, J. Dungan, and N. Cozzerelli, *Discovery of a predicted dna knot substantiates a model for site-specific recombination*, *Science* **229** (1985), no. 4709 171.
- [10] S. Alvarado, J. A. Calvo, and K. C. Millett, *The generation of random equilateral polygons*, *Journal of Statistical Physics* **143** (2011) 102–138.
- [11] J. Cantarella and C. Shonkwiler, *The symplectic geometry of closed equilateral random walks in 3-space*, .

- [12] E. J. Rawdon, *Approximating smooth thickness*, *Journal of Knot Theory and Its Ramifications* **09** (2000), no. 01 113–145,
[<http://www.worldscientific.com/doi/pdf/10.1142/S0218216500000062>].
- [13] S. Chern, *Studies in Global Geometry and Analysis*. Prentice-Hall, 1970.
- [14] K. C. Millett, M. Piatek, and E. Rawdon, *Polygonal knot space near ropelength-minimized knots*, *Journal of Knot Theory and Its Ramifications* **17** (2008), no. 05 601–631.
- [15] B. Grünbaum and J. Zaks, *Convexification of polygons by flips and by flipturns*, *Discrete Mathematics* **241** (2001), no. 13 333 – 342.
- [16] G. Toussaint, *The Erdős – Nagy theorem and its ramifications*, *Computational Geometry* **31** (2005), no. 3 219 – 236.
- [17] S. Meyn and R. Tweedie, *Markov Chains and Stochastic Stability*. Springer-Verlag, 1993.
- [18] P. G. DeGennes, *Scaling Concepts in Polymer Physics*. Cornell University Press, 1979.